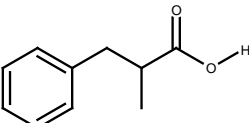
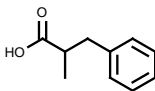


## Query

	Query	Results	Date
1. Query	 <p>Search as: As drawn, Ignore stereo, No salts</p>	15 substances	2010-09-15 12h:22m:53s (EST)

Reaxys ID 2046121 <a href="#">View in Reaxys</a>		1/15
<div></div>		<b>Chemical Name:</b> 3-phenyl-2-methylpropanoic acid; methyl-3-phenylpropionic acid; 2-benzylpropionic acid; (+/-)-2-methyl-3-phenylpropanoic acid; (+/-)-2-methyl-3-phenylpropionic acid; α-methylhydrocinnamic acid; 2-methyl-3-phenylpropanoic acid <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>CAS Registry Number:</b> 1009-67-2; 5628-72-8; 14367-54-5; 14367-67-0 <b>Molecular Weight:</b> 164.204 <b>Linear Structure Formula:</b> C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CO <sub>2</sub> H <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-UHFFFAOYSA-N <b>Note:</b>
<b>Substance Label (15)</b>		
Label	References	
5	<b>Dib, H. H.; Ibrahim, M. R.; Al-Awadi, N. A.; Ibrahim, Y. A.; Al-Awadi, S.;</b> International Journal of Chemical Kinetics; <b>vol.</b> 40; nb. 2; (2008); p. 51 - 58, <a href="#">View in Reaxys</a>	
starting to 6	<b>Reeves, Jonathan T.; Gallou, Fabrice; Song, Jinhua J.; Tan, Zhulin; Lee, Heewon; Yee, Nathan K.; Senanayake, Chris H.;</b> Tetrahedron Letters; <b>vol.</b> 48; nb. 2; (2007); p. 189 - 192, <a href="#">View in Reaxys</a>	
table 2, entry 7	<b>Oyamada, Hidekazu; Akiyama, Ryo; Hagio, Hiroyuki; Naito, Takeshi; Kobayashi, Shu;</b> Chemical Communications (Cambridge, United Kingdom); nb. 41; (2006); p. 4297 - 4299, <a href="#">View in Reaxys</a>	
Tab. 1, run 12	<b>Nakao, Ryu; Rhee, Hakjune; Uozumi, Yasuhiro;</b> Organic Letters; <b>vol.</b> 7; nb. 1; (2005); p. 163 - 165, <a href="#">View in Reaxys</a>	
2e	<b>Baan, Zoltan; Finta, Zoltan; Keglevich, Gyoergy; Hermecz, Istvan;</b> Tetrahedron Letters; <b>vol.</b> 46; nb. 37; (2005); p. 6203 - 6204, <a href="#">View in Reaxys</a>	
8	<b>Kane, John L.; Shea, Kevin M.; Crombie, Aimee L.; Danheiser, Rick L.;</b> Organic Letters; <b>vol.</b> 3; nb. 7; (2001); p. 1081 - 1084, <a href="#">View in Reaxys</a> ; <b>Joseph-McCarthy, Diane; Parris, Kevin; Huang, Adrian; Failli, Amedeo; Quagliato, Dominick; Dushin, Elizabeth Glasfeld; Novikova, Elena; Severina, Elena; Tuckman, Margareta; Petersen, Peter J.; Dean, Charles; et al. ;</b> Journal of Medicinal Chemistry; <b>vol.</b> 48; nb. 25; (2005); p. 7960 - 7969, <a href="#">View in Reaxys</a>	
58	<b>Crombie, Aimee L.; Kane, John L.; Shea, Kevin M.; Danheiser, Rick L.;</b> Journal of Organic Chemistry; <b>vol.</b> 69; nb. 25; (2004); p. 8652 - 8667, <a href="#">View in Reaxys</a>	
RPR4	<b>Verma, Raman K.; Singla, Rubina; Punniyakoti, V. T.;</b> Medicinal Chemistry Research; <b>vol.</b> 13; nb. 8-9; (2004); p. 660 - 676, <a href="#">View in Reaxys</a>	
(+/-)-8	<b>Kato, Dai-ichiro; Miyamoto, Kenji; Ohta, Hiromichi;</b> Tetrahedron: Asymmetry; <b>vol.</b> 15; nb. 18; (2004); p. 2965 - 2974, <a href="#">View in Reaxys</a>	
1b	<b>Cui, Dong-Mei; Zhang, Chen; Kawamura, Masato; Shimada, Shigeru;</b> Tetrahedron Letters; <b>vol.</b> 45; nb. 8; (2004); p. 1741 - 1746, <a href="#">View in Reaxys</a>	
15	<b>Kato, Dai-ichiro; Mitsuda, Satoshi; Ohta, Hiromichi;</b> Journal of Organic Chemistry; <b>vol.</b> 68; nb. 19; (2003); p. 7234 - 7242, <a href="#">View in Reaxys</a>	
(+/-)-4d	<b>Chandrasekhar, Sosale; Kausar, Amina;</b> Tetrahedron: Asymmetry; <b>vol.</b> 11; nb. 11; (2000); p. 2249 - 2254, <a href="#">View in Reaxys</a>	
4d	<b>Aurell, Maria Jose; Domingo, Luis Ramon; Mestres, Ramon; Munos, Elena; Zaragoza, Ramon Jose;</b> Tetrahedron; <b>vol.</b> 55; nb. 3; (1999); p. 815 - 830, <a href="#">View in Reaxys</a>	
3	<b>Lee, Mijoon; Jin, Yonghao; Kim, Dong H.;</b> Bioorganic & Medicinal Chemistry; <b>vol.</b> 7; nb. 8; (1999); p. 1755 - 1760, <a href="#">View in Reaxys</a>	
(Merck 4825)	<b>Yamamoto, Tomihiro; Matsuura, Kazuya; Shintani, Syunichi; Hara, Akira; Miyabe, Yoshiyuki; Sugiyama, Tadashi; Katagiri, Yoshihiro;</b> Biological & Pharmaceutical Bulletin; <b>vol.</b> 21; nb. 11; (1998); p. 1148 - 1153, <a href="#">View in Reaxys</a>	
<b>Patent-Specific Data (1)</b>		
Location in Patent	References	
Claim	<b>Patent; Perrine, Susan P.; Faller, Douglas V.;</b> US6011000; (2000); (A1) English, <a href="#">View in Reaxys</a> ; <b>Patent; Perrine, Susan P.;</b> US5939456; (1999); (A1) English, <a href="#">View in Reaxys</a> ; <b>Patent; Benzer, Seymour; Min, Kyung-Tai;</b> US2002/120008; (2002); (A1) English, <a href="#">View in Reaxys</a> ; <b>Patent; Beacon Laboratories, Inc.;</b> US5939455; (1999); (A1) English, <a href="#">View in Reaxys</a> ; <b>Patent; Faller, Douglas V.; Perrine, Susan P.; Stamatoynopoulos, George;</b> US2001/34367; (2001); (A1) English, <a href="#">View in Reaxys</a> ; <b>Patent; Perlmutter, David H.; Burrows, Jon A. J.; Willis, Lauren K.; Teckman, Jeffery H.;</b> US6403646; (2002); (B1) English, <a href="#">View in Reaxys</a>	

Crossfile Reference (2)				
Data Type	Name	Crossfile Source	External Access ID	References
	Benzenepropanoic acid, alpha-methyl-	CRC Handbook of Chemistry and Physics	5238	Beilstein Handbook, <a href="#">View in Reaxys</a>
13C-NMR Spectrum	A-METHYL-BENZENEPROPANOIC ACID	SpecInfo Database	STCC-50777-057 B	Unpublished, <a href="#">View in Reaxys</a>
Related Structure (1)				
Related Structure	References			
Configuration.	Watson; Youngson; Journal of the Chemical Society; (1968); p. 258,259, <a href="#">View in Reaxys</a> ; Schrecker; Journal of Organic Chemistry; vol. 22; (1957); p. 33, <a href="#">View in Reaxys</a>			
Derivative (2)				
Comment	References			
4-bromo-anilide (mp: 128-130 degree )	Hanley et al.; Journal of Organic Chemistry; vol. 23; (1958); p. 1461,1462, <a href="#">View in Reaxys</a>			
anilide (mp: 129 degree )	Shinya; Nippon Noge Kagaku Kaishi; vol. 29; (1955); p. 91,92; Chem.Abstr.; (1959); p. 1227, <a href="#">View in Reaxys</a>			
Melting Point (11)				
Melting Point [°C]	Solvent	References		
85	hexane	Suprun, W. Y.; Journal fuer Praktische Chemie/Chemiker-Zeitung; vol. 340; nb. 3; (1998); p. 247 - 255, <a href="#">View in Reaxys</a>		
34 - 36		Horner et al.; Liebigs Annalen der Chemie; (1979); p. 341,351, <a href="#">View in Reaxys</a>		
37 - 39		Byers; Wolfenden; Biochemistry; vol. 12; (1973); p. 2070, <a href="#">View in Reaxys</a>		
36 - 38		Yamada,S.; Terashima,S.; Chemical and Pharmaceutical Bulletin; vol. 16; nb. 9; (1968); p. 1816 - 1828, <a href="#">View in Reaxys</a>		
74		Patent; Farbwerke Hoechst A.G.; DE1300565; (1965); Chem.Abstr.; vol. 71; nb. 91098t; (1969), <a href="#">View in Reaxys</a>		
37	ethanol	Pastuschak; Dombrowskii; J. Gen. Chem. USSR (Engl. Transl.); vol. 34; (1964); p. 3110,3150, <a href="#">View in Reaxys</a>		
37		Patent; Shell Devel. Co.; US2010358; (1933), <a href="#">View in Reaxys</a> ; Mastagli; Lambert; Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences; vol. 233; (1951); p. 751, <a href="#">View in Reaxys</a> ; Dombrowskii et al.; Zhurnal Obshchei Khimii; vol. 27; (1957); p. 419; engl. Ausg. S. 473, <a href="#">View in Reaxys</a>		
36.6 - 37.5	pentane	Shinya; Nippon Noge Kagaku Kaishi; vol. 29; (1955); p. 91,92; Chem.Abstr.; (1959); p. 1227, <a href="#">View in Reaxys</a>		
36.5		Holden; Lapworth; Journal of the Chemical Society; (1931); p. 2368,2375, <a href="#">View in Reaxys</a>		
37.5		Willgerodt; Merk; Journal fuer Praktische Chemie (Leipzig); vol. <2> 80; (1909); p. 193, <a href="#">View in Reaxys</a>		
37	aq. ethanol	Conrad; Bischoff; Justus Liebigs Annalen der Chemie; vol. 204; (1880); p. 180, <a href="#">View in Reaxys</a>		
Boiling Point (29)				
Boiling Point [°C]	Pressure [Torr]	References		
270 - 273		Verma, Raman K.; Singla, Rubina; Punniyakoti, V. T.; Medicinal Chemistry Research; vol. 13; nb. 8-9; (2004); p. 660 - 676, <a href="#">View in Reaxys</a>		
160 - 165	22.5	Bucher, von Christoph B.; Linden, Anthony; Heimgartner, Heinz; Helvetica Chimica Acta; vol. 78; nb. 4; (1995); p. 935 - 946, <a href="#">View in Reaxys</a>		
161 - 162	16	Potapov, V. M.; Dem'yanovich, V. M.; Khlebnikov, V. A.; Zhurnal Organicheskoi Khimii; vol. 24; nb. 2; (1988); p. 343 - 348,301 - 305, <a href="#">View in Reaxys</a>		
98 - 99	0.2	Knorr, Rudolf; Lattke, Ernst; Chemische Berichte; vol. 114; nb. 6; (1981); p. 2116 - 2131, <a href="#">View in Reaxys</a>		

81 - 82	0.001	<b>Boche, Gernot; Buckl, Klaus; Martens, Diether; Schneider, Dieter R.</b> ; Liebigs Annalen der Chemie; nb. 7; (1980); p. 1135 - 1171, <a href="#">View in Reaxys</a>	
140	1	<b>Spassov; Stefanova</b> ; Journal of Molecular Structure; <b>vol.</b> 53; (1979); p. 219,220,223, <a href="#">View in Reaxys</a>	
120 - 121	1.5	<b>Kuchar et al.</b> ; Collection of Czechoslovak Chemical Communications; <b>vol.</b> 44; (1979); p. 183,186, <a href="#">View in Reaxys</a>	
92 - 94	0.02	<b>Aguir et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 41; nb. 9; (1976); p. 1545,1547, <a href="#">View in Reaxys</a>	
165	16	<b>Cocker,W.; Grayson,D.H.</b> ; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); (1975); p. 1347 - 1352, <a href="#">View in Reaxys</a>	
157	11	<b>Potapov et al.</b> ; Zhurnal Organicheskoi Khimii; <b>vol.</b> 8; (1972); p. 2319,2366,2369,2370, <a href="#">View in Reaxys</a>	
126	1.3	<b>Kashiwagi,T. et al.</b> ; Tetrahedron; <b>vol.</b> 26; (1970); p. 3619 - 3629, <a href="#">View in Reaxys</a>	
145.5	9	<b>Terashima,S. et al.</b> ; Chemical and Pharmaceutical Bulletin; <b>vol.</b> 18; (1970); p. 1124 - 1136, <a href="#">View in Reaxys</a>	
137 - 137.5	5.5	<b>Yamada,S.; Terashima,S.</b> ; Chemical and Pharmaceutical Bulletin; <b>vol.</b> 16; nb. 9; (1968); p. 1816 - 1828, <a href="#">View in Reaxys</a>	
162 - 163	13	<b>Bestmann,H.J. et al.</b> ; Chemische Berichte; <b>vol.</b> 99; (1966); p. 1906 - 1911, <a href="#">View in Reaxys</a>	
103	0.5	<b>Roberts</b> ; Journal of Organic Chemistry; <b>vol.</b> 29; (1964); p. 2714, <a href="#">View in Reaxys</a>	
146	7	<b>Urry,W.H. et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 29; nb. 7; (1964); p. 1663 - 1669, <a href="#">View in Reaxys</a>	
112 - 113	0.1	<b>Cram,D.J.; Wingrove,A.S.</b> ; Journal of the American Chemical Society; <b>vol.</b> 86; (1964); p. 5490 - 5496, <a href="#">View in Reaxys</a>	
153 - 158	10	<b>Gossauer; Ossorio</b> ; Anales de la Real Sociedad Espanola de Fisica y Quimica, Serie B: Quimica; <b>vol.</b> 59; (1963); p. 185,189, <a href="#">View in Reaxys</a>	
160 - 162	13	<b>Normant; Angelo</b> ; Bulletin de la Societe Chimique de France; (1962); p. 814, <a href="#">View in Reaxys</a>	
152 - 154	8	<b>Hjelte</b> ; Acta Chemica Scandinavica (1947-1973); <b>vol.</b> 15; (1961); p. 1200, <a href="#">View in Reaxys</a>	
150 - 152	8	<b>Marvell et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 25; (1960); p. 608,610, <a href="#">View in Reaxys</a>	
135 - 137	10	<b>Dombrowskii et al.</b> ; Zhurnal Obshchei Khimii; <b>vol.</b> 27; (1957); p. 419; engl. Ausg. S. 473, <a href="#">View in Reaxys</a>	
152 - 157	12	<b>Shinya</b> ; Nippon Nogei Kagaku Kaishi; <b>vol.</b> 29; (1955); p. 91,92; Chem.Abstr.; (1959); p. 1227, <a href="#">View in Reaxys</a>	
167 - 168	23	<b>Mastagli; Lambert</b> ; Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences; <b>vol.</b> 233; (1951); p. 751, <a href="#">View in Reaxys</a>	
160	12	<b>Kipping; Hunter</b> ; Journal of the Chemical Society; <b>vol.</b> 83; (1903); p. 1007, <a href="#">View in Reaxys</a> ; <b>Weizmann; Bergmann; Haskelberg</b> ; Chemistry and Industry (London, United Kingdom); (1937); p. 587,590, <a href="#">View in Reaxys</a>	
272 - 273		<b>Guerbet</b> ; Bulletin de la Societe Chimique de France; <b>vol.</b> <4> 3; (1908); p. 945; Chem. Zentralbl.; <b>vol.</b> 79; nb. II; (1908); p. 866, <a href="#">View in Reaxys</a> ; <b>Guerbet</b> ; Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences; <b>vol.</b> 146; (1908); p. 1406; Bulletin de la Societe Chimique de France; <b>vol.</b> <4> 3; (1908); p. 944; Chem. Zentralbl.; <b>vol.</b> 79; nb. II; (1908); p. 866, <a href="#">View in Reaxys</a>	
162	14	<b>Riiber</b> ; Chemische Berichte; <b>vol.</b> 36; (1903); p. 1406, <a href="#">View in Reaxys</a>	
160 - 161	17	<b>Kipping; Clarke</b> ; Journal of the Chemical Society; <b>vol.</b> 83; (1903); p. 916, <a href="#">View in Reaxys</a>	
272		<b>Conrad; Bischoff</b> ; Justus Liebigs Annalen der Chemie; <b>vol.</b> 204; (1880); p. 180, <a href="#">View in Reaxys</a>	
Refractive Index (6)			
Refractive Index	Wavelength [nm]	Temperature [°C]	References

1.5138	589	20	<b>Potapov et al.</b> ; Zhurnal Organicheskoi Khimii; <b>vol.</b> 8; (1972); p. 2319,2366,2369,2370, <a href="#">View in Reaxys</a>
1.5143	589	23	<b>Roberts</b> ; Journal of Organic Chemistry; <b>vol.</b> 29; (1964); p. 2714, <a href="#">View in Reaxys</a>
1.5186	589	20	<b>Urry,W.H. et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 29; nb. 7; (1964); p. 1663 - 1669, <a href="#">View in Reaxys</a>
1.5124	589	25	<b>Gossauer; Ossorio</b> ; Anales de la Real Sociedad Espanola de Fisica y Quimica, Serie B: Quimica; <b>vol.</b> 59; (1963); p. 185,189, <a href="#">View in Reaxys</a>
1.5127	589	25	<b>Gossauer; Ossorio</b> ; Anales de la Real Sociedad Espanola de Fisica y Quimica, Serie B: Quimica; <b>vol.</b> 59; (1963); p. 185,189, <a href="#">View in Reaxys</a>
1.5142	589	21	<b>Marvell et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 25; (1960); p. 608,610, <a href="#">View in Reaxys</a>
<b>Density of the Liquid (1)</b>			
Density of the Liquid	Reference Temperature [°C]	Measurement Temperature [°C]	References
1.0644	4	22	<b>Marvell et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 25; (1960); p. 608,610, <a href="#">View in Reaxys</a>
<b>Conformation (1)</b>			
Object of Investigation	References		
Conformation	<b>Spassov; Stefanova</b> ; Journal of Molecular Structure; <b>vol.</b> 53; (1979); p. 219,220,223, <a href="#">View in Reaxys</a>		
<b>Crystal Property Description (3)</b>			
Colour & Other Properties	References		
colourless	<b>Davies, Stephen G.; Hepworth, David; Roberts, Paul M.; Thomson, James E.; Goodwin, Christopher J.</b> ; Journal of Organic Chemistry; <b>vol.</b> 75; nb. 4; (2010); p. 1214 - 1227, <a href="#">View in Reaxys</a>		
colourless	<b>Alcalde, Ermitas; Mesquida, Neus; Lopez-Perez, Sara; Frigola, Jordi; Merce, Ramon</b> ; Organic and Bio-molecular Chemistry; <b>vol.</b> 6; nb. 20; (2008); p. 3795 - 3810, <a href="#">View in Reaxys</a>		
Blaetter	<b>Conrad; Bischoff</b> ; Justus Liebigs Annalen der Chemie; <b>vol.</b> 204; (1880); p. 180, <a href="#">View in Reaxys</a>		
<b>Optical Rotatory Power (6)</b>			
1 of 6	Type	[alpha]	
	Optical Rotatory Power [deg]	1.78	
	Wavelength [nm]	589	
	<b>Horner et al.</b> ; Liebigs Annalen der Chemie; (1979); p. 341,351, <a href="#">View in Reaxys</a>		
2 of 6	Type	[alpha]	
	Optical Rotatory Power [deg]	0.97	
	Wavelength [nm]	589	
	<b>Horner et al.</b> ; Liebigs Annalen der Chemie; (1979); p. 341,351, <a href="#">View in Reaxys</a>		
3 of 6	Type	[alpha]	
	Optical Rotatory Power [deg]	0.36	
	Wavelength [nm]	436	
	<b>Horner et al.</b> ; Liebigs Annalen der Chemie; (1979); p. 341,351, <a href="#">View in Reaxys</a>		
4 of 6	Type	[alpha]	
	Optical Rotatory Power [deg]	0.86	
	Wavelength [nm]	436	

	<b>Horner et al.</b> ; Liebigs Annalen der Chemie; (1979); p. 341,351, <a href="#">View in Reaxys</a>	
5 of 6	Type	[alpha]
	Optical Rotatory Power [deg]	17.9
	Wavelength [nm]	589
	<b>Aviron-Violet et al.</b> ; Journal of Molecular Catalysis; <b>vol. 5</b> ; (1979); p. 44; Chem.Abstr.; <b>vol. 91</b> ; nb. 57462k, <a href="#">View in Reaxys</a>	
6 of 6	Type	[alpha]
	Optical Rotatory Power [deg]	4.3
	Wavelength [nm]	589
	Temperature [°C]	21
	<b>Aguir et al.</b> ; Journal of Organic Chemistry; <b>vol. 41</b> ; nb. 9; (1976); p. 1545,1547, <a href="#">View in Reaxys</a>	
<b>Dissociation Exponent (2)</b>		
1 of 2	Comment	(pk')pK: 6.95 (25grad, 88percent Methylcellosolve, potentiometrisch)
	<b>Kuchar et al.</b> ; Cesko-Slovenska Farmacie; <b>vol. 29</b> ; (1980); p. 281, <a href="#">View in Reaxys</a>	
2 of 2	Comment	(pk')pK
	<b>Kuchar et al.</b> ; Collection of Czechoslovak Chemical Communications; <b>vol. 44</b> ; (1979); p. 183,186, <a href="#">View in Reaxys</a>	
<b>Further Information (1)</b>		
Description		References
Further information	<b>Beamer; Lawson</b> ; Journal of Pharmaceutical Sciences; <b>vol. 55</b> ; (1966); p. 53,55, <a href="#">View in Reaxys</a> ; <b>Marshall et al.</b> ; Journal of Organic Chemistry; <b>vol. 31</b> ; (1966); p. 4315,4317, <a href="#">View in Reaxys</a>	
<b>Solubility (MCS) (1)</b>		
1 of 1	Temperature [°C]	15
	Solvent	H2O
	Comment	0.309 part(s) of substance.dissolves in:100 parts of solvent.
	<b>Conrad; Bischoff</b> ; Justus Liebigs Annalen der Chemie; <b>vol. 204</b> ; (1880); p. 180, <a href="#">View in Reaxys</a>	
<b>NMR Spectroscopy (15)</b>		
1 of 15	Description	Chemical shifts
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	200
	<b>Davies, Stephen G.; Hepworth, David; Roberts, Paul M.; Thomson, James E.; Goodwin, Christopher J.</b> ; Journal of Organic Chemistry; <b>vol. 75</b> ; nb. 4; (2010); p. 1214 - 1227, <a href="#">View in Reaxys</a>	
2 of 15	Description	Chemical shifts
	Nucleus	13C
	Solvents	CDCl3
	<b>Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John</b> ; Tetrahedron; <b>vol. 52</b> ; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a> ; <b>Jamie, Joanne F.; Rickards, Rodney W.</b> ; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); nb. 21; (1996); p. 2603 - 2614, <a href="#">View in Reaxys</a> ; <b>Suprun, W. Y.</b> ; Journal fuer Praktische Chemie/Chemiker-Zeitung; <b>vol. 340</b> ; nb. 3; (1998); p. 247 - 255, <a href="#">View in Reaxys</a> ; <b>Dib, H. H.; Ibrahim, M. R.; Al-Awadi, N. A.; Ibrahim, Y. A.; Al-Awadi, S.</b> ; International Journal of Chemical Kinetics; <b>vol. 40</b> ; nb. 2; (2008); p. 51 - 58, <a href="#">View in Reaxys</a>	
3 of 15	Description	Chemical shifts
	Nucleus	1H
	Solvents	CDCl3
	Frequency [MHz]	400

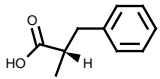
	<b>Dib, H. H.; Ibrahim, M. R.; Al-Awadi, N. A.; Ibrahim, Y. A.; Al-Awadi, S.</b> ; International Journal of Chemical Kinetics; <b>vol. 40</b> ; nb. 2; (2008); p. 51 - 58, <a href="#">View in Reaxys</a> ; <b>Fox, Martin E.; Jackson, Mark; Lennon, Ian C.; Klosin, Jerzy; Abboud, Khalil A.</b> ; Journal of Organic Chemistry; <b>vol. 73</b> ; nb. 3; (2008); p. 775 - 784, <a href="#">View in Reaxys</a>	
4 of 15	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
	Solvents	chloroform-d1
	Temperature [°C]	24.84
	Frequency [MHz]	300
	<b>Alcalde, Ermitas; Mesquida, Neus; Lopez-Perez, Sara; Frigola, Jordi; Merce, Ramon</b> ; Organic and Biomolecular Chemistry; <b>vol. 6</b> ; nb. 20; (2008); p. 3795 - 3810, <a href="#">View in Reaxys</a>	
5 of 15	Description	Chemical shifts
	Nucleus	<sup>13</sup> C
	Solvents	chloroform-d1
	Temperature [°C]	24.84
	Frequency [MHz]	75.4
	<b>Alcalde, Ermitas; Mesquida, Neus; Lopez-Perez, Sara; Frigola, Jordi; Merce, Ramon</b> ; Organic and Biomolecular Chemistry; <b>vol. 6</b> ; nb. 20; (2008); p. 3795 - 3810, <a href="#">View in Reaxys</a>	
6 of 15	Description	Chemical shifts
	Nucleus	<sup>13</sup> C
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Aurell, Maria Jose; Domingo, Luis Ramon; Mestres, Ramon; Munos, Elena; Zaragoza, Ramon Jose</b> ; Tetrahedron; <b>vol. 55</b> ; nb. 3; (1999); p. 815 - 830, <a href="#">View in Reaxys</a>	
7 of 15	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Aurell, Maria Jose; Domingo, Luis Ramon; Mestres, Ramon; Munos, Elena; Zaragoza, Ramon Jose</b> ; Tetrahedron; <b>vol. 55</b> ; nb. 3; (1999); p. 815 - 830, <a href="#">View in Reaxys</a>	
8 of 15	Nucleus	<sup>1</sup> H
	Coupling Nuclei	<sup>1</sup> H
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Aurell, Maria Jose; Domingo, Luis Ramon; Mestres, Ramon; Munos, Elena; Zaragoza, Ramon Jose</b> ; Tetrahedron; <b>vol. 55</b> ; nb. 3; (1999); p. 815 - 830, <a href="#">View in Reaxys</a>	
9 of 15	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
	Solvents	CDCl <sub>3</sub>
	<b>Stamm, Helmut; Sommer, Andreas; Onistschenko, Andreas; Woderer, Anton</b> ; Journal of Organic Chemistry; <b>vol. 51</b> ; nb. 25; (1986); p. 4979 - 4983, <a href="#">View in Reaxys</a> ; <b>Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John</b> ; Tetrahedron; <b>vol. 52</b> ; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a> ; <b>Jamie, Joanne F.; Rickards, Rodney W.</b> ; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); nb. 21; (1996); p. 2603 - 2614, <a href="#">View in Reaxys</a> ; <b>Suprun, W. Y.</b> ; Journal fuer Praktische Chemie/Chemiker-Zeitung; <b>vol. 340</b> ; nb. 3; (1998); p. 247 - 255, <a href="#">View in Reaxys</a>	
10 of 15	Description	Spin-spin coupling constants
	Solvents	CDCl <sub>3</sub>
	Comment	<sup>1</sup> H- <sup>1</sup> H



	<b>Stamm, Helmut; Sommer, Andreas; Onitschenko, Andreas; Woderer, Anton</b> ; Journal of Organic Chemistry; <b>vol.</b> 51; nb. 25; (1986); p. 4979 - 4983, <a href="#">View in Reaxys</a> ; <b>Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John</b> ; Tetrahedron; <b>vol.</b> 52; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a> ; <b>Jamie, Joanne F.; Rickards, Rodney W.</b> ; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); nb. 21; (1996); p. 2603 - 2614, <a href="#">View in Reaxys</a>		
11 of 15	Description	Chemical shifts	
	Nucleus	1H	
	Solvents	CDCl3	
	Temperature [°C]	26.9	
	<b>Bucher, von Christoph B.; Linden, Anthony; Heimgartner, Heinz</b> ; Helvetica Chimica Acta; <b>vol.</b> 78; nb. 4; (1995); p. 935 - 946, <a href="#">View in Reaxys</a>		
12 of 15	Description	Spin-spin coupling constants	
	Solvents	CDCl3	
	Temperature [°C]	26.9	
	Comment	1H-1H.	
	<b>Bucher, von Christoph B.; Linden, Anthony; Heimgartner, Heinz</b> ; Helvetica Chimica Acta; <b>vol.</b> 78; nb. 4; (1995); p. 935 - 946, <a href="#">View in Reaxys</a>		
13 of 15	Description	Chemical shifts	
	Nucleus	1H	
	Solvents	CCl4	
	<b>Boche, Gernot; Buckl, Klaus; Martens, Diether; Schneider, Dieter R.</b> ; Liebigs Annalen der Chemie; nb. 7; (1980); p. 1135 - 1171, <a href="#">View in Reaxys</a> ; <b>Kawashima, Masatoshi; Sato, Toshio; Fujisawa, Tamotsu</b> ; Tetrahedron; <b>vol.</b> 45; nb. 2; (1989); p. 403 - 412, <a href="#">View in Reaxys</a> ; <b>Knorr, Rudolf; Lattke, Ernst</b> ; Chemische Berichte; <b>vol.</b> 114; nb. 6; (1981); p. 2116 - 2131, <a href="#">View in Reaxys</a>		
14 of 15	Description	Spin-spin coupling constants	
	Solvents	CCl4	
	Comment	1H-1H	
	<b>Boche, Gernot; Buckl, Klaus; Martens, Diether; Schneider, Dieter R.</b> ; Liebigs Annalen der Chemie; nb. 7; (1980); p. 1135 - 1171, <a href="#">View in Reaxys</a> ; <b>Kawashima, Masatoshi; Sato, Toshio; Fujisawa, Tamotsu</b> ; Tetrahedron; <b>vol.</b> 45; nb. 2; (1989); p. 403 - 412, <a href="#">View in Reaxys</a> ; <b>Knorr, Rudolf; Lattke, Ernst</b> ; Chemische Berichte; <b>vol.</b> 114; nb. 6; (1981); p. 2116 - 2131, <a href="#">View in Reaxys</a>		
15 of 15	Description	NMR	
	<b>Spassov; Stefanova</b> ; Journal of Molecular Structure; <b>vol.</b> 53; (1979); p. 219,220,223, <a href="#">View in Reaxys</a> ; <b>Jaouen; Dabard</b> ; Bulletin de la Societe Chimique de France; (1974); p. 1646,1649, <a href="#">View in Reaxys</a>		
<b>IR Spectroscopy (8)</b>			
Description	Solvent	Comment	References
Bands		film	<b>Alcalde, Ermitas; Mesquida, Neus; Lopez-Perez, Sara; Frigola, Jordi; Merce, Ramon</b> ; Organic and Biomolecular Chemistry; <b>vol.</b> 6; nb. 20; (2008); p. 3795 - 3810, <a href="#">View in Reaxys</a>
Bands	film		<b>Kato, Dai-ichiro; Mitsuda, Satoshi; Ohta, Hiromichi</b> ; Journal of Organic Chemistry; <b>vol.</b> 68; nb. 19; (2003); p. 7234 - 7242, <a href="#">View in Reaxys</a>
Bands	NaCl	3420 - 1693 cm <sup>-1</sup>	<b>Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John</b> ; Tetrahedron; <b>vol.</b> 52; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a>
Bands	neat (no solvent)	3400 - 695 cm <sup>-1</sup>	<b>Jamie, Joanne F.; Rickards, Rodney W.</b> ; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); nb. 21; (1996); p. 2603 - 2614, <a href="#">View in Reaxys</a>
Bands	neat (no solvent)	3025 - 700 cm <sup>-1</sup>	<b>Bucher, von Christoph B.; Linden, Anthony; Heimgartner, Heinz</b> ; Helvetica Chimica Acta; <b>vol.</b> 78; nb. 4; (1995); p. 935 - 946, <a href="#">View in Reaxys</a>



Bands	neat (no solvent)	3090 - 700 cm**(-1)	<b>Kawashima, Masatoshi; Sato, Toshio; Fujisawa, Tamotsu</b> ; Tetra- hedron; <b>vol.</b> 45; nb. 2; (1989); p. 403 - 412, <a href="#">View in Reaxys</a>
Bands	neat (no solvent)	1705 cm**(-1)	<b>Stamm, Helmut; Sommer, Andreas; Onitschenko, Andreas; Wo- derer, Anton</b> ; Journal of Organic Chemistry; <b>vol.</b> 51; nb. 25; (1986); p. 4979 - 4983, <a href="#">View in Reaxys</a>
Bands			<b>Yamada,S.; Terashima,S.</b> ; Chemical and Pharmaceutical Bulletin; <b>vol.</b> 16; nb. 9; (1968); p. 1816 - 1828, <a href="#">View in Reaxys</a>
<b>Mass Spectrometry (3)</b>			
Description	References		
spectrum	<b>Suprun, W. Y.</b> ; Journal fuer Praktische Chemie/Chemiker-Zeitung; <b>vol.</b> 340; nb. 3; (1998); p. 247 - 255, <a href="#">View in Reaxys</a> ; <b>Dib, H. H.; Ibrahim, M. R.; Al-Awadi, N. A.; Ibrahim, Y. A.; Al-Awadi, S.</b> ; International Journal of Chemical Kinetics; <b>vol.</b> 40; nb. 2; (2008); p. 51 - 58, <a href="#">View in Reaxys</a>		
EI (Electron im- pact); Spectrum	<b>Alcalde, Ermitas; Mesquida, Neus; Lopez-Perez, Sara; Frigola, Jordi; Merce, Ramon</b> ; Organic and Bio- molecular Chemistry; <b>vol.</b> 6; nb. 20; (2008); p. 3795 - 3810, <a href="#">View in Reaxys</a>		
spectrum; elec- tron impact (EI)	<b>Jamie, Joanne F.; Rickards, Rodney W.</b> ; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); nb. 21; (1996); p. 2603 - 2614, <a href="#">View in Reaxys</a>		
<b>UV/VIS Spectroscopy (1)</b>			
Description	Solvent	Comment	References
Spectrum	propan-2-ol	230 - 340 nm	<b>Shinya</b> ; Nippon Nogei Kagaku Kaishi; <b>vol.</b> 29; (1955); p. 91,92; Chem.Abstr.; (1959); p. 1227, <a href="#">View in Reaxys</a>
<b>Pharmacological Data (1)</b>			
1 of 1	Effect	enzyme; examination of	
	Species or Test-System	human liver S-indan-1-ol dehydrogenase (AKR1C4)	
	Concentration	20 - 1000 µmol/l	
	Method	enzyme incub. with title comp. + 2.0 mmol/l S-indan-1-ol + 0.25 mmol/l NADP(+) in phos- phate buffer (pH 7.4); enzyme activity (EA) assayed fluorometrically or spectrophotometri- cally	
	Further Details	title comp. effect on EA studied	
	Results	biphasic response: stimulation of EA at 20-500 µmol/l; inhibition of EA at 500-1000 µmol/l (graph)	
	<b>Yamamoto, Tomihiro; Matsuura, Kazuya; Shintani, Syunichi; Hara, Akira; Miyabe, Yoshiyuki; Sugiyama, Ta- dashi; Katagiri, Yoshihiro</b> ; Biological & Pharmaceutical Bulletin; <b>vol.</b> 21; nb. 11; (1998); p. 1148 - 1153, <a href="#">View in Reaxys</a>		

Reaxys ID 2614110 <a href="#">View in Reaxys</a>		2/15
		<p><b>Chemical Name:</b> (S)-(+)-α-methyldihydrocinnamic acid; (2S)-(+)-2-methyl-3-phenyl propanoic acid; (S)-(+)-α-methylhydrocinnamic acid; (S)-α-methylbenzenepropanoic acid; (2S)-2-Methyl-3-phenylpropanoic acid; (2S)-2-methyl-3-phenylpropionic acid; (S)-2-Methyl-3-phenylpropionic acid</p> <p><b>Molecular Formula:</b> C<sub>10</sub>H<sub>12</sub>O<sub>2</sub></p> <p><b>CAS Registry Number:</b> 1009-67-2; 5628-72-8; 14367-54-5; 14367-67-0</p> <p><b>Molecular Weight:</b> 164.204</p> <p><b>Linear Structure Formula:</b> C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>CHCH<sub>3</sub>CO<sub>2</sub>H</p> <p><b>Type of Substance:</b> isocyclic</p> <p><b>InChIKey:</b> MCIIDRLDHRQKPH-QMMMGPBSA-N</p> <p><b>Note:</b></p>
<b>Substance Label (22)</b>		
Label	References	
(S)-11c	<b>Green, Rachel; Merritt, Andrew T.; Bull, Steven D.</b> ; Chemical Communications (Cambridge, United Kingdom); nb. 4; (2008); p. 508 - 510, <a href="#">View in Reaxys</a>	
S acid	<b>Kuil, Mark; Goudriaan, P. Elsbeth; Kleij, Arjan W.; Tooke, Duncan M.; Spek, Anthony L.; Leeuwen, Piet W. N. M. van; Reek, Joost N. H.</b> ; Dalton Transactions; nb. 22; (2007); p. 2311 - 2320, <a href="#">View in Reaxys</a>	

(S)-10	<b>Suzuki, Takayoshi; Hisakawa, Shinya; Itoh, Yukihiro; Maruyama, Sakiko; Kurotaki, Mineko; Nakagawa, Hidehiko; Miyata, Naoki;</b> Bioorganic & Medicinal Chemistry Letters; <b>vol.</b> 17; nb. 6; (2007); p. 1558 - 1561, <a href="#">View in Reaxys</a>
21	<b>McGhee, Andrea M.; Kizirian, Jean-Claude; Procter, David J.;</b> Organic and Biomolecular Chemistry; <b>vol.</b> 5; nb. 7; (2007); p. 1021 - 1024, <a href="#">View in Reaxys</a>
(S)-5e, Tab. 1, run 27	<b>Qiu, Liqin; Li, Yue-Ming; Kwong, Fuk Yee; Yu, Wing-Yiu; Fan, Qing-Hua; Chan, Albert S. C.;</b> Advanced Synthesis and Catalysis; <b>vol.</b> 349; nb. 4-5; (2007); p. 517 - 520, <a href="#">View in Reaxys</a>
9c	<b>Le, Thanh Nguyen; Nguyen, Quynh Pham Bao; Kim, Jae Nyoung; Kim, Taek Hyeon;</b> Tetrahedron Letters; <b>vol.</b> 48; nb. 44; (2007); p. 7834 - 7837, <a href="#">View in Reaxys</a>
(S)-5a	<b>Cheng, Xu; Xie, Jian-Hua; Li, Sheng; Zhou, Qi-Lin;</b> Advanced Synthesis and Catalysis; <b>vol.</b> 348; nb. 10-11; (2006); p. 1271 - 1276, <a href="#">View in Reaxys</a>
42	<b>Davies, Stephen G.; Garner, A. Christopher; Roberts, Paul M.; Smith, Andrew D.; Sweet, Miles J.; Thomson, James E.;</b> Organic and Biomolecular Chemistry; <b>vol.</b> 4; nb. 14; (2006); p. 2753 - 2768, <a href="#">View in Reaxys</a>
(S)-14	<b>Tessier, Arnaud; Pytkowicz, Julien; Brigaud, Thierry;</b> Angewandte Chemie, International Edition; <b>vol.</b> 45; nb. 22; (2006); p. 3677 - 3681; Angewandte Chemie; <b>vol.</b> 118; nb. 22; (2006); p. 3759 - 3763, <a href="#">View in Reaxys</a>
3	<b>Allin, Steven M.; Johnson, Cara A.; Timm, Andreas;</b> Tetrahedron Letters; <b>vol.</b> 46; nb. 14; (2005); p. 2495 - 2498, <a href="#">View in Reaxys</a>
26a	<b>Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki;</b> Tetrahedron; <b>vol.</b> 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a>
2	<b>Hoen, Rob; Boogers, Jeroen A. F.; Bernsmann, Heiko; Minnaard, Adriaan J.; Meetsma, Auke; Tiemersma-Wegman, Theodora D.; Vries, Andre H. M. de; Vries, Johannes G. de; Feringa, Ben L. ;</b> Angewandte Chemie, International Edition; <b>vol.</b> 44; nb. 27; (2005); p. 4209 - 4212; Angewandte Chemie; <b>vol.</b> 117; nb. 27; (2005); p. 4281 - 4284, <a href="#">View in Reaxys</a>
(S)-8	<b>Kato, Dai-ichiro; Miyamoto, Kenji; Ohta, Hiromichi;</b> Tetrahedron: Asymmetry; <b>vol.</b> 15; nb. 18; (2004); p. 2965 - 2974, <a href="#">View in Reaxys</a>
3b	<b>Srivastava, Stuti; Goswami, Lalit N.; Dikshit, Dinesh K.;</b> Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry; <b>vol.</b> 42; nb. 10; (2003); p. 2628 - 2631, <a href="#">View in Reaxys</a>
Tab. 1, entry 12	<b>Sturm, Thomas; Weissensteiner, Walter; Spindler, Felix;</b> Advanced Synthesis and Catalysis; <b>vol.</b> 345; nb. 1-2; (2003); p. 160 - 164, <a href="#">View in Reaxys</a>
32	<b>Davies, Stephen G.; Dixon, Darren J.; Doisneau, Gilles J.-M.; Prodger, Jeremy C.; Sanganee, Hitesh J.;</b> Tetrahedron: Asymmetry; <b>vol.</b> 13; nb. 6; (2002); p. 647 - 658, <a href="#">View in Reaxys</a>
18-(S)	<b>Maienza, Francesca; Santoro, Francesco; Spindler, Felix; Malan, Christophe; Mezzetti, Antonio;</b> Tetrahedron: Asymmetry; <b>vol.</b> 13; nb. 16; (2002); p. 1817 - 1824, <a href="#">View in Reaxys</a>
(S)-17H2	<b>Maienza, Francesca; Spindler, Felix; Thommen, Marc; Pugin, Benoit; Malan, Christophe; Mezzetti, Antonio;</b> Journal of Organic Chemistry; <b>vol.</b> 67; nb. 15; (2002); p. 5239 - 5249, <a href="#">View in Reaxys</a>
25	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Lecumberri, Ainara; Linden, Anthony ;</b> Organic Letters; <b>vol.</b> 3; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a>
28	<b>Alexander, Karen; Cook, Stuart; Gibson, Colin L.; Kennedy, Alan R.;</b> Journal of the Chemical Society, Perkin Transactions 1; nb. 13; (2001); p. 1538 - 1549, <a href="#">View in Reaxys</a>
19	<b>Bull, Steven D.; Davies, Stephen G.; Jones, Simon; Sanganee, Hitesh J.;</b> Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); nb. 4; (1999); p. 387 - 398, <a href="#">View in Reaxys</a>
5	<b>Townsend, Craig A.; Neese, A. Scott; Theis, Alan B.;</b> Journal of the Chemical Society, Chemical Communications; nb. 2; (1982); p. 116 - 118, <a href="#">View in Reaxys</a>
<b>Related Structure (1)</b>	
Related Structure	References
Configuration.	<b>Watson; Youngson;</b> Journal of the Chemical Society; (1968); p. 258,259, <a href="#">View in Reaxys</a> ; <b>Schrecker;</b> Journal of Organic Chemistry; <b>vol.</b> 22; (1957); p. 33, <a href="#">View in Reaxys</a>
<b>Derivative (1)</b>	
Comment	References
quinine salt (mp: 122-118 degree , mp: 116-110 degree , mp: 109 de-	<b>Kenyon; Ross;</b> Journal of the Chemical Society; (1951); p. 3407,3409, <a href="#">View in Reaxys</a> ; <b>Akabori; Sakurai;</b> Nippon Kagaku Zasshi; <b>vol.</b> 78; (1957); p. 1629; Chem.Abstr.; (1959); p. 21687, <a href="#">View in Reaxys</a> ; <b>Nerdel; John;</b> Chemische Berichte; <b>vol.</b> 89; (1956); p. 1945,1949, <a href="#">View in Reaxys</a>

gree ; <al-pha>=-111.2 de- gree ); Further Da- ta see Handbook			
Purification (2)			
Purification (meth- od)	References		
(-)-α-phenethyla- mine	Terashima,S. et al.; Chemical and Pharmaceutical Bulletin; vol. 18; (1970); p. 1124 - 1136, <a href="#">View in Reaxys</a>		
quinine	Cram,D.J.; Wingrove,A.S.; Journal of the American Chemical Society; vol. 86; (1964); p. 5490 - 5496, <a href="#">View in Reaxys</a> ; Watson,M.B.; Youngson,G.W.; Journal of the Chemical Society [Section] C: Organic; (1968); p. 258 - 262, <a href="#">View in Reaxys</a>		
Boiling Point (10)			
Boiling Point [°C]	Pressure [Torr]	Comment	References
100	2		Oetvoes, Laszlo; Kraicsovits, Ferenc; Tetrahedron; vol. 48; nb. 23; (1992); p. 5009 - 5014, <a href="#">View in Reaxys</a>
96 - 98	1		Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C.; Journal of Organic Chemistry; vol. 56; nb. 10; (1991); p. 3286 - 3294, <a href="#">View in Reaxys</a>
138 - 140	3		Kobayashi,M. et al.; Chemical and Pharmaceutical Bulletin; vol. 20; (1972); p. 1898 - 1905, <a href="#">View in Reaxys</a>
142 - 144	5		Terashima,S. et al.; Chemical and Pharmaceutical Bulletin; vol. 18; (1970); p. 1124 - 1136, <a href="#">View in Reaxys</a>
125 - 126	1.5		Cram,D.J.; Wingrove,A.S.; Journal of the American Chemical Soci- ety; vol. 86; (1964); p. 5490 - 5496, <a href="#">View in Reaxys</a>
112	0.3		Schrecker; Journal of Organic Chemistry; vol. 22; (1957); p. 33, <a href="#">View in Reaxys</a>
142 - 145	6		Akabori; Sakurai; Nippon Kagaku Zasshi; vol. 78; (1957); p. 1629; Chem.Abstr.; (1959); p. 21687, <a href="#">View in Reaxys</a>
167 - 169	23		Kenyon; Ross; Journal of the Chemical Society; (1951); p. 3407,3409, <a href="#">View in Reaxys</a>
150	1		Levene; Marker; Journal of Biological Chemistry; vol. 110; (1935); p. 299,303, <a href="#">View in Reaxys</a>
160	13	Oel.	Pickard; Yates; Journal of the Chemical Society; vol. 95; (1909); p. 1018, <a href="#">View in Reaxys</a>
Refractive Index (2)			
Refractive Index	Wavelength [nm]	Temperature [°C]	References
1.5126	589	25	Kenyon; Ross; Journal of the Chemical Society; (1951); p. 3407,3409, <a href="#">View in Reaxys</a>
1.5008	589	24	Kenyon; Phillips; Pittman; Journal of the Chemical Society; (1935); p. 1079, <a href="#">View in Reaxys</a>
Density of the Liquid (3)			
Density of the Liq- uid	Reference Tem- perature [°C]	Measurement Temperature [°C]	References
1.062	4	20	Nerdel; John; Chemische Berichte; vol. 89; (1956); p. 1945,1949, <a href="#">View in Reaxys</a>
1.062	4	24	Kenyon; Phillips; Pittman; Journal of the Chemical Society; (1935); p. 1079, <a href="#">View in Reaxys</a>
1.065	4	20	Pickard; Yates; Journal of the Chemical Society; vol. 95; (1909); p. 1018, <a href="#">View in Reaxys</a>
Crystal Property Description (2)			
Colour & Other Properties	References		
colourless	Li, Shen; Zhu, Shou-Fei; Zhang, Can-Ming; Song, Song; Zhou, Qi-Lin; Journal of the American Chemical Society; vol. 130; nb. 27; (2008); p. 8584 - 8585, <a href="#">View in Reaxys</a>		

light-yellow	<b>McGhee, Andrea M.; Kizirian, Jean-Claude; Procter, David J.</b> ; Organic and Biomolecular Chemistry; <b>vol. 5</b> ; nb. 7; (2007); p. 1021 - 1024, <a href="#">View in Reaxys</a>	
<b>Optical Rotatory Power (47)</b>		
1 of 47	Type	[alpha]
	Concentration	1 g/100ml
	Solvent	chloroform
	Optical Rotatory Power [deg]	21.3
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Zupancic, Borut; Mohar, Barbara; Stephan, Michel</b> ; Organic Letters; <b>vol. 12</b> ; nb. 13; (2010); p. 3022 - 3025, <a href="#">View in Reaxys</a>	
2 of 47	Type	[alpha]
	Concentration	0.82 g/100ml
	Solvent	chloroform
	Optical Rotatory Power [deg]	30.2
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Li, Shen; Zhu, Shou-Fei; Zhang, Can-Ming; Song, Song; Zhou, Qi-Lin</b> ; Journal of the American Chemical Society; <b>vol. 130</b> ; nb. 27; (2008); p. 8584 - 8585, <a href="#">View in Reaxys</a>	
3 of 47	Type	[alpha]
	Concentration	0.19 g/100ml
	Solvent	CHCl3
	Optical Rotatory Power [deg]	24.2
	Wavelength [nm]	589
	Temperature [°C]	24
	<b>Le, Thanh Nguyen; Nguyen, Quynh Pham Bao; Kim, Jae Nyoung; Kim, Taek Hyeon</b> ; Tetrahedron Letters; <b>vol. 48</b> ; nb. 44; (2007); p. 7834 - 7837, <a href="#">View in Reaxys</a>	
4 of 47	Type	[alpha]
	Concentration	0.6 g/100ml
	Length of Path [cm]	10
	Solvent	CHCl3
	Optical Rotatory Power [deg]	26.8
	Wavelength [nm]	589
	Temperature [°C]	25
<b>Davies, Stephen G.; Garner, A. Christopher; Roberts, Paul M.; Smith, Andrew D.; Sweet, Miles J.; Thomson, James E.</b> ; Organic and Biomolecular Chemistry; <b>vol. 4</b> ; nb. 14; (2006); p. 2753 - 2768, <a href="#">View in Reaxys</a>		
5 of 47	Type	[alpha]
	Concentration	1.0 g/100ml
	Solvent	CHCl3
	Optical Rotatory Power [deg]	28.6
	Wavelength [nm]	589
	Temperature [°C]	21

	<b>Davies, Stephen G.; Dixon, Darren J.; Doisneau, Gilles J.-M.; Prodger, Jeremy C.; Sanganee, Hitesh J.;</b> Tetrahedron: Asymmetry; <b>vol.</b> 13; nb. 6; (2002); p. 647 - 658, <a href="#">View in Reaxys</a>	
6 of 47	Type	[alpha]
	Concentration	1.0 g/100ml
	Solvent	CH <sub>2</sub> Cl <sub>2</sub>
	Optical Rotatory Power [deg]	29
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Le-cumberri, Ainara; Linden, Anthony</b> ; Organic Letters; <b>vol.</b> 3; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a>	
7 of 47	Type	[alpha]
	Concentration	1 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	-26.5
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Bull, Steven D.; Davies, Stephen G.; Jones, Simon; Sanganee, Hitesh J.;</b> Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); nb. 4; (1999); p. 387 - 398, <a href="#">View in Reaxys</a>	
8 of 47	Type	[alpha]
	Concentration	0.95 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	24.6
	Wavelength [nm]	589
	<b>Ghosh, Arun K.; Cho, Hanna; Onishi, Masanobu;</b> Tetrahedron: Asymmetry; <b>vol.</b> 8; nb. 6; (1997); p. 821 - 824, <a href="#">View in Reaxys</a>	
9 of 47	Type	[alpha]
	Concentration	1.0 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	27
	Wavelength [nm]	589
	<b>Ferorelli, S.; Loiodice, F.; Tortorella, V.; Amoroso, R.; Bettoni, G.; et al.;</b> Farmaco; <b>vol.</b> 52; nb. 6/7; (1997); p. 367 - 374, <a href="#">View in Reaxys</a>	
10 of 47	Type	[alpha]
	Concentration	5.5 g/100ml
	Solvent	ethanol
	Optical Rotatory Power [deg]	23.81
	Wavelength [nm]	589
	Temperature [°C]	22
	<b>Allin, Steven M.; Shuttleworth, Stephen J.;</b> Tetrahedron Letters; <b>vol.</b> 37; nb. 44; (1996); p. 8023 - 8026, <a href="#">View in Reaxys</a>	
11 of 47	Type	[alpha]
	Concentration	1 g/100ml

	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	30.4
	Wavelength [nm]	589
	Temperature [°C]	21
	<b>Davies, Stephen G.; Sanganee, Hitesh J.</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 6; nb. 3; (1995); p. 671 - 674, <a href="#">View in Reaxys</a>	
12 of 47	Type	[alpha]
	Concentration	0.8 g/100ml
	Solvent	benzene
	Optical Rotatory Power [deg]	25
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Sibi, Mukund P.; Deshpande, Prasad K.; Ji, Jianguo</b> ; Tetrahedron Letters; <b>vol.</b> 36; nb. 49; (1995); p. 8965 - 8968, <a href="#">View in Reaxys</a>	
13 of 47	Type	[alpha]
	Concentration	3 g/100ml
	Solvent	benzene
	Optical Rotatory Power [deg]	26.65
	Wavelength [nm]	589
	<b>Oetvoes, Laszlo; Kraicsovits, Ferenc</b> ; Tetrahedron; <b>vol.</b> 48; nb. 23; (1992); p. 5009 - 5014, <a href="#">View in Reaxys</a>	
14 of 47	Type	[alpha]
	Concentration	2.37 g/100ml
	Solvent	ethanol
	Optical Rotatory Power [deg]	17.7
	Wavelength [nm]	589
	<b>Chu, Kent S.; Negrete, George R.; Konopelski, Joseph P.; Lakner, Frederick J.; Woo, Nam-Tae; Olmstead, Marilyn M.</b> ; Journal of the American Chemical Society; <b>vol.</b> 114; nb. 5; (1992); p. 1800 - 1812, <a href="#">View in Reaxys</a>	
15 of 47	Type	[alpha]
	Concentration	1 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	25.5
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Oppolzer, Wolfgang; Lienard, Philippe</b> ; Helvetica Chimica Acta; <b>vol.</b> 75; nb. 8; (1992); p. 2572 - 2582, <a href="#">View in Reaxys</a>	
16 of 47	Type	[alpha]
	Concentration	1 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	26.5 - 85.9
	Wavelength [nm]	365 - 578

	Temperature [°C]	20
	<b>Oppolzer, Wolfgang; Lienard, Philippe</b> ; Helvetica Chimica Acta; <b>vol.</b> 75; nb. 8; (1992); p. 2572 - 2582, <a href="#">View in Reaxys</a>	
17 of 47	Type	[alpha]
	Concentration	4 g/100ml
	Solvent	ethanol
	Optical Rotatory Power [deg]	21.54
	Wavelength [nm]	589
	Temperature [°C]	23
	<b>Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C.</b> ; Journal of Organic Chemistry; <b>vol.</b> 56; nb. 10; (1991); p. 3286 - 3294, <a href="#">View in Reaxys</a>	
18 of 47	Type	[alpha]
	Concentration	1.006 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	25.74
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Colombo, M.; Amici, M. De; Micheli, C. De; Pitre, D.; Carrea, G.; Riva, S.</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 2; nb. 10; (1991); p. 1021 - 1030, <a href="#">View in Reaxys</a>	
19 of 47	Type	[alpha]
	Concentration	0.85 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	28.3
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Oppolzer, Wolfgang; Rodriguez, Ines; Starkemann, Christian; Walther, Eric</b> ; Tetrahedron Letters; <b>vol.</b> 31; nb. 35; (1990); p. 5019 - 5022, <a href="#">View in Reaxys</a>	
20 of 47	Type	[alpha]
	Concentration	1 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	25.6
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Delnick, Deborah L.; Margolin, Alexey L.</b> ; Tetrahedron Letters; <b>vol.</b> 31; nb. 47; (1990); p. 6797 - 6798, <a href="#">View in Reaxys</a>	
21 of 47	Type	[alpha]
	Concentration	1.15 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	29.3
	Wavelength [nm]	589
	Temperature [°C]	20



	<b>Oppolzer, Wolfgang; Moretti, Robert; Thomi, Silvia</b> ; Tetrahedron Letters; <b>vol.</b> 30; nb. 41; (1989); p. 5603 - 5606, <a href="#">View in Reaxys</a>	
22 of 47	Type	[alpha]
	Concentration	0.87 g/100ml
	Solvent	ethanol
	Optical Rotatory Power [deg]	21
	Wavelength [nm]	589
	Temperature [°C]	26
	<b>Kawanami, Yasuhiro; Ito, Yoshio; Kitagawa, Toshiyuki; Taniguchi, Yoshiyuki; Katsuki, Tsutomu; Yamaguchi, Masaru</b> ; Tetrahedron Letters; <b>vol.</b> 25; nb. 8; (1984); p. 857 - 860, <a href="#">View in Reaxys</a>	
23 of 47	Type	[alpha]
	Optical Rotatory Power [deg]	25.2
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Guoqiang, Lin; Hjalmarsson, Mats; Hoegberg, Hans-Erik; Jernstedt, Karen; Norin, Torbjoern</b> ; Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry; <b>vol.</b> 38; nb. 9; (1984); p. 795 - 802, <a href="#">View in Reaxys</a>	
24 of 47	Type	[alpha]
	Concentration	5.78 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	29.6
	Wavelength [nm]	589
	Temperature [°C]	22
	<b>Townsend, Craig A.; Neese, A. Scott; Theis, Alan B.</b> ; Journal of the Chemical Society, Chemical Communications; nb. 2; (1982); p. 116 - 118, <a href="#">View in Reaxys</a>	
25 of 47	Type	alpha
	Length of Path [cm]	1
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	2.693
	Wavelength [nm]	589
	Temperature [°C]	19.5
	<b>Kobayashi, M. et al.</b> ; Chemical and Pharmaceutical Bulletin; <b>vol.</b> 20; (1972); p. 1898 - 1905, <a href="#">View in Reaxys</a>	
26 of 47	Type	alpha
	Length of Path [cm]	1
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	2.686
	Wavelength [nm]	589
	Temperature [°C]	19
	<b>Terashima, S. et al.</b> ; Chemical and Pharmaceutical Bulletin; <b>vol.</b> 18; (1970); p. 1124 - 1136, <a href="#">View in Reaxys</a>	
27 of 47	Type	[alpha]
	Concentration	5.346 g/100ml
	Solvent	CHCl <sub>3</sub>

	Optical Rotatory Power [deg]	29.3
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Terashima,S. et al.</b> ; Chemical and Pharmaceutical Bulletin; <b>vol.</b> 18; (1970); p. 1124 - 1136, <a href="#">View in Reaxys</a>	
28 of 47	Type	[alpha]
	Concentration	5.810 g/100ml
	Solvent	benzene
	Optical Rotatory Power [deg]	31.5
	Wavelength [nm]	589
	Temperature [°C]	16
	<b>Terashima,S. et al.</b> ; Chemical and Pharmaceutical Bulletin; <b>vol.</b> 18; (1970); p. 1124 - 1136, <a href="#">View in Reaxys</a>	
29 of 47	Type	[alpha]
	Concentration	1.12 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	26.3
	Wavelength [nm]	589
	Temperature [°C]	27
	<b>Cohen,S.G.; Milovanovic,A.</b> ; Journal of the American Chemical Society; <b>vol.</b> 90; (1968); p. 3495 - 3502, <a href="#">View in Reaxys</a>	
30 of 47	Type	alpha
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	20.4
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Watson,M.B.; Youngson,G.W.</b> ; Journal of the Chemical Society [Section] C: Organic; (1968); p. 258 - 262, <a href="#">View in Reaxys</a>	
31 of 47	Type	alpha
	Length of Path [cm]	10
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	22.92
	Wavelength [nm]	589
	Temperature [°C]	26
	<b>Cram,D.J.; Wingrove,A.S.</b> ; Journal of the American Chemical Society; <b>vol.</b> 86; (1964); p. 5490 - 5496, <a href="#">View in Reaxys</a>	
32 of 47	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	23.5
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Schrecker</b> ; Journal of Organic Chemistry; <b>vol.</b> 22; (1957); p. 33, <a href="#">View in Reaxys</a>	

33 of 47	Type	[alpha]
	Concentration	c=3.7
	Solvent	benzene
	Optical Rotatory Power [deg]	24
	Wavelength [nm]	589
	Temperature [°C]	29
	<b>Akabori; Sakurai</b> ; Nippon Kagaku Zasshi; <b>vol.</b> 78; (1957); p. 1629; Chem.Abstr.; (1959); p. 21687, <a href="#">View in Reaxys</a>	
34 of 47	Type	[alpha]
	Concentration	c=0.033
	Solvent	ethanol
	Optical Rotatory Power [deg]	11.5
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>DeTar; Weis</b> ; Journal of the American Chemical Society; <b>vol.</b> 79; (1957); p. 30, <a href="#">View in Reaxys</a>	
35 of 47	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	22.9
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Nerdel; John</b> ; Chemische Berichte; <b>vol.</b> 89; (1956); p. 1945,1949, <a href="#">View in Reaxys</a>	
36 of 47	Type	alpha
	Length of Path [cm]	10
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	13.4
	Wavelength [nm]	589
	Temperature [°C]	19
	<b>Kenyon; Ross</b> ; Journal of the Chemical Society; (1951); p. 3407,3409, <a href="#">View in Reaxys</a>	
37 of 47	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	20.4
	Wavelength [nm]	589
	Temperature [°C]	24
	<b>Levene; Marker</b> ; Journal of Biological Chemistry; <b>vol.</b> 110; (1935); p. 299,303, <a href="#">View in Reaxys</a>	
38 of 47	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	19.1
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Levene; Marker</b> ; Journal of Biological Chemistry; <b>vol.</b> 110; (1935); p. 299,303, <a href="#">View in Reaxys</a>	

39 of 47	Type	[alpha]
	Concentration	c=5
	Solvent	ethanol
	Optical Rotatory Power [deg]	17.9
	Wavelength [nm]	589
	Temperature [°C]	21
	<b>Kenyon; Phillips; Pittman</b> ; Journal of the Chemical Society; (1935); p. 1079, <a href="#">View in Reaxys</a>	
40 of 47	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	24.8
	Wavelength [nm]	546
	Temperature [°C]	24
	<b>Kenyon; Phillips; Pittman</b> ; Journal of the Chemical Society; (1935); p. 1079, <a href="#">View in Reaxys</a>	
41 of 47	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	45.4
	Wavelength [nm]	436
	Temperature [°C]	24
	<b>Kenyon; Phillips; Pittman</b> ; Journal of the Chemical Society; (1935); p. 1079, <a href="#">View in Reaxys</a>	
42 of 47	Type	[alpha]
	Concentration	c=5
	Solvent	ethanol
	Optical Rotatory Power [deg]	44.5
	Wavelength [nm]	436
	Temperature [°C]	21
	<b>Kenyon; Phillips; Pittman</b> ; Journal of the Chemical Society; (1935); p. 1079, <a href="#">View in Reaxys</a>	
43 of 47	Type	alpha
	Length of Path [cm]	10
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	-9.56
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Jones; Wallis</b> ; Journal of the American Chemical Society; <b>vol. 48</b> ; (1926); p. 180, <a href="#">View in Reaxys</a>	
44 of 47	Type	[alpha]
	Optical Rotatory Power [deg]	22.65
	Wavelength [nm]	589
	<b>Pickard; Yates</b> ; Journal of the Chemical Society; <b>vol. 95</b> ; (1909); p. 1018, <a href="#">View in Reaxys</a>	
45 of 47	Type	[alpha]

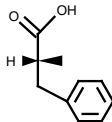
	Optical Rotatory Power [deg]	27.06
	Wavelength [nm]	589
	<b>Pickard; Yates</b> ; Journal of the Chemical Society; <b>vol.</b> 95; (1909); p. 1018, <a href="#">View in Reaxys</a>	
46 of 47	Type	[alpha]
	Optical Rotatory Power [deg]	27.72
	Wavelength [nm]	589
	<b>Pickard; Yates</b> ; Journal of the Chemical Society; <b>vol.</b> 95; (1909); p. 1018, <a href="#">View in Reaxys</a>	
47 of 47	Type	[alpha]
	Optical Rotatory Power [deg]	22.65
	Wavelength [nm]	589
	Comment	im ungelosten Zustand.
	<b>Pickard; Yates</b> ; Journal of the Chemical Society; <b>vol.</b> 95; (1909); p. 1018, <a href="#">View in Reaxys</a>	
<b>Optical Rotatory Dispersion (1)</b>		
Comment		References
656.3 - 486.1 nm		<b>Nerdel; John</b> ; Chemische Berichte; <b>vol.</b> 89; (1956); p. 1945,1949, <a href="#">View in Reaxys</a>
<b>NMR Spectroscopy (19)</b>		
1 of 19	Description	Chemical shifts
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	300
	<b>Zupancic, Borut; Mohar, Barbara; Stephan, Michel</b> ; Organic Letters; <b>vol.</b> 12; nb. 13; (2010); p. 3022 - 3025, <a href="#">View in Reaxys</a>	
2 of 19	Description	Chemical shifts
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	400
	<b>Li, Shen; Zhu, Shou-Fei; Zhang, Can-Ming; Song, Song; Zhou, Qi-Lin</b> ; Journal of the American Chemical Society; <b>vol.</b> 130; nb. 27; (2008); p. 8584 - 8585, <a href="#">View in Reaxys</a>	
3 of 19	Description	Chemical shifts
	Nucleus	1H
	Solvents	CDCl3
	Frequency [MHz]	500
	<b>McGhee, Andrea M.; Kizirian, Jean-Claude; Procter, David J.</b> ; Organic and Biomolecular Chemistry; <b>vol.</b> 5; nb. 7; (2007); p. 1021 - 1024, <a href="#">View in Reaxys</a>	
4 of 19	Nucleus	1H
	Coupling Nuclei	1H
	Solvents	CDCl3
	Frequency [MHz]	500
	<b>McGhee, Andrea M.; Kizirian, Jean-Claude; Procter, David J.</b> ; Organic and Biomolecular Chemistry; <b>vol.</b> 5; nb. 7; (2007); p. 1021 - 1024, <a href="#">View in Reaxys</a>	
5 of 19	Description	Chemical shifts
	Nucleus	1H
	Solvents	CDCl3

	Frequency [MHz]	400
	<b>Davies, Stephen G.; Garner, A. Christopher; Roberts, Paul M.; Smith, Andrew D.; Sweet, Miles J.; Thomson, James E.</b> ; Organic and Biomolecular Chemistry; <b>vol.</b> 4; nb. 14; (2006); p. 2753 - 2768, <a href="#">View in Reaxys</a>	
6 of 19	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	250
	<b>Tessier, Arnaud; Pytkowicz, Julien; Brigaud, Thierry</b> ; Angewandte Chemie, International Edition; <b>vol.</b> 45; nb. 22; (2006); p. 3677 - 3681; Angewandte Chemie; <b>vol.</b> 118; nb. 22; (2006); p. 3759 - 3763, <a href="#">View in Reaxys</a>	
7 of 19	Description	Chemical shifts
	Nucleus	<sup>13</sup> C
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	62.9
	<b>Tessier, Arnaud; Pytkowicz, Julien; Brigaud, Thierry</b> ; Angewandte Chemie, International Edition; <b>vol.</b> 45; nb. 22; (2006); p. 3677 - 3681; Angewandte Chemie; <b>vol.</b> 118; nb. 22; (2006); p. 3759 - 3763, <a href="#">View in Reaxys</a>	
8 of 19	Nucleus	<sup>1</sup> H
	Coupling Nuclei	<sup>1</sup> H
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	300
	<b>Davies, Stephen G.; Dixon, Darren J.; Doisneau, Gilles J.-M.; Prodger, Jeremy C.; Sangane, Hitesh J.</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 13; nb. 6; (2002); p. 647 - 658, <a href="#">View in Reaxys</a> ; <b>Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki</b> ; Tetrahedron; <b>vol.</b> 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a>	
9 of 19	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	300
	<b>Davies, Stephen G.; Dixon, Darren J.; Doisneau, Gilles J.-M.; Prodger, Jeremy C.; Sangane, Hitesh J.</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 13; nb. 6; (2002); p. 647 - 658, <a href="#">View in Reaxys</a> ; <b>Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki</b> ; Tetrahedron; <b>vol.</b> 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a>	
10 of 19	Description	Spectrum
	Nucleus	<sup>1</sup> H
	<b>Allin, Steven M.; Johnson, Cara A.; Timm, Andreas</b> ; Tetrahedron Letters; <b>vol.</b> 46; nb. 14; (2005); p. 2495 - 2498, <a href="#">View in Reaxys</a>	
11 of 19	Description	Chemical shifts
	Nucleus	<sup>13</sup> C
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	75.5
	<b>Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki</b> ; Tetrahedron; <b>vol.</b> 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a>	
12 of 19	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Ho, Rob; Boegers, Jeroen A. F.; Bernsmann, Heiko; Minnaard, Adriaan J.; Meetsma, Auke; Tiemersma-Wegman, Theodora D.; Vries, Andre H. M. de; Vries, Johannes G. de; Feringa, Ben L.</b> ; Angewandte Chemie, Inter-	

	national Edition; <b>vol.</b> 44; nb. 27; (2005); p. 4209 - 4212; Angewandte Chemie; <b>vol.</b> 117; nb. 27; (2005); p. 4281 - 4284, <a href="#">View in Reaxys</a>	
13 of 19	Nucleus	1H
	Coupling Nuclei	1H
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Hoën, Rob; Boogers, Jeroen A. F.; Bernsmann, Heiko; Minnaard, Adriaan J.; Meetsma, Auke; Tiemersma-Wegman, Theodora D.; Vries, Andre H. M. de; Vries, Johannes G. de; Feringa, Ben L.</b> ; Angewandte Chemie, International Edition; <b>vol.</b> 44; nb. 27; (2005); p. 4209 - 4212; Angewandte Chemie; <b>vol.</b> 117; nb. 27; (2005); p. 4281 - 4284, <a href="#">View in Reaxys</a>	
14 of 19	Description	Chemical shifts
	Nucleus	13C
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	50.32
	<b>Hoën, Rob; Boogers, Jeroen A. F.; Bernsmann, Heiko; Minnaard, Adriaan J.; Meetsma, Auke; Tiemersma-Wegman, Theodora D.; Vries, Andre H. M. de; Vries, Johannes G. de; Feringa, Ben L.</b> ; Angewandte Chemie, International Edition; <b>vol.</b> 44; nb. 27; (2005); p. 4209 - 4212; Angewandte Chemie; <b>vol.</b> 117; nb. 27; (2005); p. 4281 - 4284, <a href="#">View in Reaxys</a>	
15 of 19	Description	Chemical shifts
	Nucleus	1H
	Solvents	CDCl <sub>3</sub>
	<b>Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C.</b> ; Journal of Organic Chemistry; <b>vol.</b> 56; nb. 10; (1991); p. 3286 - 3294, <a href="#">View in Reaxys</a> ; <b>Chu, Kent S.; Negrete, George R.; Konopelski, Joseph P.; Lakner, Frederick J.; Woo, Nam-Tae; Olmstead, Marilyn M.</b> ; Journal of the American Chemical Society; <b>vol.</b> 114; nb. 5; (1992); p. 1800 - 1812, <a href="#">View in Reaxys</a> ; <b>Oppolzer, Wolfgang; Lienard, Philippe</b> ; Helvetica Chimica Acta; <b>vol.</b> 75; nb. 8; (1992); p. 2572 - 2582, <a href="#">View in Reaxys</a> ; <b>Ferorelli, S.; Loiodice, F.; Tortorella, V.; Amoroso, R.; Bettoni, G.; et al.</b> ; Farmaco; <b>vol.</b> 52; nb. 6/7; (1997); p. 367 - 374, <a href="#">View in Reaxys</a> ; <b>Srivastava, Stuti; Goswami, Lalit N.; Dikshit, Dinesh K.</b> ; Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry; <b>vol.</b> 42; nb. 10; (2003); p. 2628 - 2631, <a href="#">View in Reaxys</a>	
16 of 19	Description	Chemical shifts
	Nucleus	13C
	Solvents	CDCl <sub>3</sub>
	<b>Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C.</b> ; Journal of Organic Chemistry; <b>vol.</b> 56; nb. 10; (1991); p. 3286 - 3294, <a href="#">View in Reaxys</a> ; <b>Chu, Kent S.; Negrete, George R.; Konopelski, Joseph P.; Lakner, Frederick J.; Woo, Nam-Tae; Olmstead, Marilyn M.</b> ; Journal of the American Chemical Society; <b>vol.</b> 114; nb. 5; (1992); p. 1800 - 1812, <a href="#">View in Reaxys</a> ; <b>Srivastava, Stuti; Goswami, Lalit N.; Dikshit, Dinesh K.</b> ; Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry; <b>vol.</b> 42; nb. 10; (2003); p. 2628 - 2631, <a href="#">View in Reaxys</a>	
17 of 19	Nucleus	1H
	Coupling Nuclei	1H
	Solvents	CDCl <sub>3</sub>
	<b>Srivastava, Stuti; Goswami, Lalit N.; Dikshit, Dinesh K.</b> ; Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry; <b>vol.</b> 42; nb. 10; (2003); p. 2628 - 2631, <a href="#">View in Reaxys</a>	
18 of 19	Description	Chemical shifts
	Nucleus	1H
	Coupling Nuclei	1H
	Solvents	CDCl <sub>3</sub>
	<b>Bull, Steven D.; Davies, Stephen G.; Jones, Simon; Sangane, Hitesh J.</b> ; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999); nb. 4; (1999); p. 387 - 398, <a href="#">View in Reaxys</a>	
19 of 19	Description	Spin-spin coupling constants
	Solvents	CDCl <sub>3</sub>
	Comment	1H-1H



<b>Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C.;</b> Journal of Organic Chemistry; <b>vol.</b> 56; nb. 10; (1991); p. 3286 - 3294, <a href="#">View in Reaxys</a> ; <b>Chu, Kent S.; Negrete, George R.; Konopelski, Joseph P.; Lakner, Frederick J.; Woo, Nam-Tae; Olmstead, Marilyn M.;</b> Journal of the American Chemical Society; <b>vol.</b> 114; nb. 5; (1992); p. 1800 - 1812, <a href="#">View in Reaxys</a> ; <b>Oppolzer, Wolfgang; Lienard, Philippe;</b> Helvetica Chimica Acta; <b>vol.</b> 75; nb. 8; (1992); p. 2572 - 2582, <a href="#">View in Reaxys</a>			
<b>IR Spectroscopy (3)</b>			
Description	Solvent	Comment	References
Bands	neat liquid		<b>Srivastava, Stuti; Goswami, Lalit N.; Dikshit, Dinesh K.;</b> Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry; <b>vol.</b> 42; nb. 10; (2003); p. 2628 - 2631, <a href="#">View in Reaxys</a> ; <b>McGhee, Andrea M.; Kizirian, Jean-Claude; Procter, David J.;</b> Organic and Biomolecular Chemistry; <b>vol.</b> 5; nb. 7; (2007); p. 1021 - 1024, <a href="#">View in Reaxys</a>
Bands	neat (no solvent)	1700 cm <sup>**</sup> (-1)	<b>Ferorelli, S.; Loiodice, F.; Tortorella, V.; Amoroso, R.; Bettoni, G.; et al.;</b> Farmaco; <b>vol.</b> 52; nb. 6/7; (1997); p. 367 - 374, <a href="#">View in Reaxys</a>
Bands	neat (no solvent)	3400 - 1703 cm <sup>**</sup> (-1)	<b>Chu, Kent S.; Negrete, George R.; Konopelski, Joseph P.; Lakner, Frederick J.; Woo, Nam-Tae; Olmstead, Marilyn M.;</b> Journal of the American Chemical Society; <b>vol.</b> 114; nb. 5; (1992); p. 1800 - 1812, <a href="#">View in Reaxys</a>
<b>Mass Spectrometry (1)</b>			
Description	References		
spectrum	<b>Ferorelli, S.; Loiodice, F.; Tortorella, V.; Amoroso, R.; Bettoni, G.; et al.;</b> Farmaco; <b>vol.</b> 52; nb. 6/7; (1997); p. 367 - 374, <a href="#">View in Reaxys</a>		
<b>Rotational Spectroscopy (1)</b>			
Description	Comment	References	
Rotational spectrum	Rotationsdispersion (Heptan; 405-587 mμ):.	<b>Rothen; Levene;</b> Journal of Chemical Physics; 7 <1939< 975, 977, <a href="#">View in Reaxys</a>	

Reaxys ID 2502292 <a href="#">View in Reaxys</a>		3/15
		<p><b>Chemical Name:</b> (R)-(-)-α-methylhydrocinnamic acid; (R)-(-)-2-methyl-3-phenylpropionic acid; (2R)-2-methyl-3-phenylpropionic acid; (R)-2-Methyl-3-phenylpropionic acid; (R)-2-methyl-3-phenylpropanoic acid; (-)-(2R)-methylhydrocinnamic acid; 2-methyl-3-phenylpropionic acid</p> <p><b>Molecular Formula:</b> C<sub>10</sub>H<sub>12</sub>O<sub>2</sub></p> <p><b>CAS Registry Number:</b> 14367-67-0; 5628-72-8; 14367-54-5; 1009-67-2</p> <p><b>Molecular Weight:</b> 164.204</p> <p><b>Linear Structure Formula:</b> C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>CHCH<sub>3</sub>CO<sub>2</sub>H</p> <p><b>Type of Substance:</b> isocyclic</p> <p><b>InChIKey:</b> MCIIDRLDHRQKPH-MRVPVSSYSA-N</p> <p><b>Note:</b></p>
<b>Substance Label (20)</b>		
Label	References	
(R)-11a	<b>Green, Rachel; Merritt, Andrew T.; Bull, Steven D.;</b> Chemical Communications (Cambridge, United Kingdom); nb. 4; (2008); p. 508 - 510, <a href="#">View in Reaxys</a>	
R acid	<b>Kuil, Mark; Goudriaan, P. Elsbeth; Kleij, Arjan W.; Tooke, Duncan M.; Spek, Anthony L.; Leeuwen, Piet W. N. M. van; Reek, Joost N. H.;</b> Dalton Transactions; nb. 22; (2007); p. 2311 - 2320, <a href="#">View in Reaxys</a>	
(R)-10	<b>Suzuki, Takayoshi; Hisakawa, Shinya; Itoh, Yukihiro; Maruyama, Sakiko; Kurotaki, Mineko; Nakagawa, Hidehiko; Miyata, Naoki;</b> Bioorganic & Medicinal Chemistry Letters; <b>vol.</b> 17; nb. 6; (2007); p. 1558 - 1561, <a href="#">View in Reaxys</a>	
(R)-5e, Tab. 1, run 27	<b>Qiu, Liqin; Li, Yue-Ming; Kwong, Fuk Yee; Yu, Wing-Yiu; Fan, Qing-Hua; Chan, Albert S. C.;</b> Advanced Synthesis and Catalysis; <b>vol.</b> 349; nb. 4-5; (2007); p. 517 - 520, <a href="#">View in Reaxys</a>	
9a	<b>Le, Thanh Nguyen; Nguyen, Quynh Pham Bao; Kim, Jae Nyoung; Kim, Taek Hyeon;</b> Tetrahedron Letters; <b>vol.</b> 48; nb. 44; (2007); p. 7834 - 7837, <a href="#">View in Reaxys</a>	

(R)-5a	<b>Cheng, Xu; Xie, Jian-Hua; Li, Sheng; Zhou, Qi-Lin</b> ; Advanced Synthesis and Catalysis; <b>vol.</b> 348; nb. 10-11; (2006); p. 1271 - 1276, <a href="#">View in Reaxys</a>		
40	<b>Davies, Stephen G.; Garner, A. Christopher; Roberts, Paul M.; Smith, Andrew D.; Sweet, Miles J.; Thomson, James E.</b> ; Organic and Biomolecular Chemistry; <b>vol.</b> 4; nb. 14; (2006); p. 2753 - 2768, <a href="#">View in Reaxys</a>		
26f	<b>Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki</b> ; Tetrahedron; <b>vol.</b> 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a>		
2, enantiomer	<b>Hoën, Rob; Boogers, Jeroen A. F.; Bernsmann, Heiko; Minnaard, Adriaan J.; Meetsma, Auke; Tiemersma-Wegman, Theodora D.; Vries, Andre H. M. de; Vries, Johannes G. de; Feringa, Ben L.</b> ; Angewandte Chemie, International Edition; <b>vol.</b> 44; nb. 27; (2005); p. 4209 - 4212; Angewandte Chemie; <b>vol.</b> 117; nb. 27; (2005); p. 4281 - 4284, <a href="#">View in Reaxys</a>		
(R)-8	<b>Kato, Dai-ichiro; Miyamoto, Kenji; Ohta, Hiromichi</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 15; nb. 18; (2004); p. 2965 - 2974, <a href="#">View in Reaxys</a>		
ent-3b	<b>Srivastava, Stuti; Goswami, Lalit N.; Dikshit, Dinesh K.</b> ; Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry; <b>vol.</b> 42; nb. 10; (2003); p. 2628 - 2631, <a href="#">View in Reaxys</a>		
Tab. 1, entry 12	<b>Sturm, Thomas; Weissensteiner, Walter; Spindler, Felix</b> ; Advanced Synthesis and Catalysis; <b>vol.</b> 345; nb. 1-2; (2003); p. 160 - 164, <a href="#">View in Reaxys</a>		
18-(R)	<b>Maienza, Francesca; Santoro, Francesco; Spindler, Felix; Malan, Christophe; Mezzetti, Antonio</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 13; nb. 16; (2002); p. 1817 - 1824, <a href="#">View in Reaxys</a>		
9	<b>Yang, Qifei; Olmsted, Courtney; Borhan, Babak</b> ; Organic Letters; <b>vol.</b> 4; nb. 20; (2002); p. 3423 - 3426, <a href="#">View in Reaxys</a>		
(R)-17H2	<b>Maienza, Francesca; Spindler, Felix; Thommen, Marc; Pugin, Benoit; Malan, Christophe; Mezzetti, Antonio</b> ; Journal of Organic Chemistry; <b>vol.</b> 67; nb. 15; (2002); p. 5239 - 5249, <a href="#">View in Reaxys</a>		
26	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Lecumberri, Ainara; Linden, Anthony</b> ; Organic Letters; <b>vol.</b> 3; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a>		
27	<b>Alexander, Karen; Cook, Stuart; Gibson, Colin L.; Kennedy, Alan R.</b> ; Journal of the Chemical Society, Perkin Transactions 1; nb. 13; (2001); p. 1538 - 1549, <a href="#">View in Reaxys</a>		
4d	<b>Chandrasekhar, Sosale; Kausar, Amina</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 11; nb. 11; (2000); p. 2249 - 2254, <a href="#">View in Reaxys</a>		
60	<b>Hintermann, Tobias; Seebach, Dieter</b> ; Helvetica Chimica Acta; <b>vol.</b> 81; nb. 11; (1998); p. 2093 - 2126, <a href="#">View in Reaxys</a>		
(R)-(-)-III	<b>Potatov, V. M.; Dem'yanovich, V. M.; Vendrova, O. E.; Strel'tsova, E. S.</b> ; Journal of Organic Chemistry USSR (English Translation); <b>vol.</b> 17; nb. 11; (1981); p. 2080 - 2083; Zhurnal Organicheskoi Khimii; <b>vol.</b> 17; nb. 11; (1981); p. 2329 - 2333, <a href="#">View in Reaxys</a>		
Related Structure (1)			
Related Structure	References		
Configuration.	<b>Watson; Youngson</b> ; Journal of the Chemical Society; (1968); p. 258,259, <a href="#">View in Reaxys</a> ; <b>Schrecker</b> ; Journal of Organic Chemistry; <b>vol.</b> 22; (1957); p. 33, <a href="#">View in Reaxys</a>		
Boiling Point (6)			
Boiling Point [°C]	Pressure [Torr]	References	
122 - 125	1	<b>Potatov, V. M.; Dem'yanovich, V. M.; Vendrova, O. E.; Strel'tsova, E. S.</b> ; Journal of Organic Chemistry USSR (English Translation); <b>vol.</b> 17; nb. 11; (1981); p. 2080 - 2083; Zhurnal Organicheskoi Khimii; <b>vol.</b> 17; nb. 11; (1981); p. 2329 - 2333, <a href="#">View in Reaxys</a> ; <b>Potapov, V. M.; Dem'yanovich, V. M; Vendrova, O. E.; Khlebnikov, V. A.</b> ; Zhurnal Organicheskoi Khimii; <b>vol.</b> 18; nb. 6; (1982); p. 1205 - 1208,1041 - 1043, <a href="#">View in Reaxys</a>	
114	0.3	<b>Bezmer; Brown</b> ; Journal of Pharmaceutical Sciences; <b>vol.</b> 60; (1971); p. 583,584, <a href="#">View in Reaxys</a>	
111	0.2	<b>Schrecker</b> ; Journal of Organic Chemistry; <b>vol.</b> 22; (1957); p. 33, <a href="#">View in Reaxys</a>	
123 - 124	1.5	<b>DeTar; Weis</b> ; Journal of the American Chemical Society; <b>vol.</b> 79; (1957); p. 3045,3048, <a href="#">View in Reaxys</a>	
150 - 152	8	<b>Bhide; Sudborough</b> ; Journal of the Indian Institute of Science; <b>vol.</b> 8; (1925); p. 96; Chem. Zentralbl.; <b>vol.</b> 97; nb. I; (1926); p. 80, <a href="#">View in Reaxys</a>	
155 - 156	11	<b>Kay; Raper</b> ; Biochemical Journal; <b>vol.</b> 18; (1924); p. 157, <a href="#">View in Reaxys</a>	
Refractive Index (1)			
Refractive Index	Wavelength [nm]	Temperature [°C]	References

1.5145	589	20	<b>Schrecker</b> ; Journal of Organic Chemistry; <b>vol.</b> 22; (1957); p. 33, <a href="#">View in Reaxys</a>
<b>Density of the Liquid (1)</b>			
Density of the Liquid	Reference Temperature [°C]	Measurement Temperature [°C]	References
1.065	4	22	<b>Schrecker</b> ; Journal of Organic Chemistry; <b>vol.</b> 22; (1957); p. 33, <a href="#">View in Reaxys</a>
<b>Crystal Property Description (1)</b>			
Colour & Other Properties	References		
colorless	<b>Patent</b> ; <b>DOW GLOBAL TECHNOLOGIES INC.</b> ; WO2007/123957; (2007); (A2) English, <a href="#">View in Reaxys</a>		
<b>Optical Rotatory Power (21)</b>			
1 of 21	Type	[alpha]	
	Concentration	1.0 g/100ml	
	Solvent	CHCl3	
	Optical Rotatory Power [deg]	-25	
	Wavelength [nm]	589	
	Temperature [°C]	21	
	<b>Green, Rachel; Merritt, Andrew T.; Bull, Steven D.</b> ; Chemical Communications (Cambridge, United Kingdom); nb. 4; (2008); p. 508 - 510, <a href="#">View in Reaxys</a>		
2 of 21	Type	[alpha]	
	Concentration	0.17 g/100ml	
	Solvent	CHCl3	
	Optical Rotatory Power [deg]	-24	
	Wavelength [nm]	589	
	Temperature [°C]	24	
	<b>Le, Thanh Nguyen; Nguyen, Quynh Pham Bao; Kim, Jae Nyoung; Kim, Taek Hyeon</b> ; Tetrahedron Letters; <b>vol.</b> 48; nb. 44; (2007); p. 7834 - 7837, <a href="#">View in Reaxys</a>		
3 of 21	Type	[alpha]	
	Concentration	1.02 g/100ml	
	Solvent	chloroform	
	Optical Rotatory Power [deg]	-22.7	
	Wavelength [nm]	589	
	Temperature [°C]	25	
	<b>Patent</b> ; <b>DOW GLOBAL TECHNOLOGIES INC.</b> ; WO2007/123957; (2007); (A2) English, <a href="#">View in Reaxys</a>		
4 of 21	Type	[alpha]	
	Concentration	0.8 g/100ml	
	Length of Path [cm]	10	
	Solvent	CHCl3	
	Optical Rotatory Power [deg]	-21.6	
	Wavelength [nm]	589	
	Temperature [°C]	20	
	<b>Davies, Stephen G.; Garner, A. Christopher; Roberts, Paul M.; Smith, Andrew D.; Sweet, Miles J.; Thomson, James E.</b> ; Organic and Biomolecular Chemistry; <b>vol.</b> 4; nb. 14; (2006); p. 2753 - 2768, <a href="#">View in Reaxys</a>		

5 of 21	Type	[alpha]
	Concentration	1.04 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	-30.7
	Wavelength [nm]	589
	Temperature [°C]	28
	<b>Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshia-ki; Tetrahedron; vol. 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a></b>	
6 of 21	Type	[alpha]
	Concentration	0.8 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	-23.6
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Lee, Gue-Jae; Kim, Taek Hyeon; Kim, Jae Nyoung; Lee, Uk; Tetrahedron: Asymmetry; vol. 13; nb. 1; (2002); p. 9 - 12, <a href="#">View in Reaxys</a></b>	
7 of 21	Type	[alpha]
	Concentration	1.0 g/100ml
	Solvent	CH <sub>2</sub> Cl <sub>2</sub>
	Optical Rotatory Power [deg]	-29.5
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Le-cumberri, Ainara; Linden, Anthony ; Organic Letters; vol. 3; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a></b>	
8 of 21	Type	[alpha]
	Concentration	0.12 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	-26.1
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Alexander, Karen; Cook, Stuart; Gibson, Colin L.; Kennedy, Alan R.; Journal of the Chemical Society, Perkin Transactions 1; nb. 13; (2001); p. 1538 - 1549, <a href="#">View in Reaxys</a></b>	
9 of 21	Type	[alpha]
	Concentration	1.1 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	-25.9
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Hintermann, Tobias; Seebach, Dieter; Helvetica Chimica Acta; vol. 81; nb. 11; (1998); p. 2093 - 2126, <a href="#">View in Reaxys</a></b>	
10 of 21	Type	[alpha]

	Concentration	7.66 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	-27.3
	Wavelength [nm]	589
	Temperature [°C]	19.2
	<b>Sudo, Atsushi; Saigo, Kazuhiko</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 6; nb. 9; (1995); p. 2153 - 2156, <a href="#">View in Reaxys</a> ; <b>Sudo, Atsushi; Saigo, Kazuhiko</b> ; Tetrahedron: Asymmetry; <b>vol.</b> 7; nb. 10; (1996); p. 2939 - 2956, <a href="#">View in Reaxys</a>	
11 of 21	Type	[alpha]
	Concentration	1 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	-23.1
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John</b> ; Tetrahedron; <b>vol.</b> 52; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a>	
12 of 21	Type	[alpha]
	Concentration	0.90 g/100ml
	Solvent	CH <sub>2</sub> Cl <sub>2</sub>
	Optical Rotatory Power [deg]	-29.7
	Wavelength [nm]	589
	Temperature [°C]	22
	<b>Tanner, David; Birgersson, Carin; Gogoll, Adolf; Luthman, Kristina</b> ; Tetrahedron; <b>vol.</b> 50; nb. 32; (1994); p. 9797 - 9824, <a href="#">View in Reaxys</a>	
13 of 21	Type	[alpha]
	Concentration	0.27 g/100ml
	Solvent	methanol
	Optical Rotatory Power [deg]	-16.7
	Wavelength [nm]	589
	Temperature [°C]	23
	<b>Wilson, Kenneth E.; Burk, Robert M.; Biftu, Tesfaye; Ball, Richard G.; Hoogsteen, Karst</b> ; Journal of Organic Chemistry; <b>vol.</b> 57; nb. 28; (1992); p. 7151 - 7158, <a href="#">View in Reaxys</a>	
14 of 21	Type	[alpha]
	Concentration	1 g/100ml
	Solvent	CHCl <sub>3</sub>
	Optical Rotatory Power [deg]	-26.2
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Delnick, Deborah L.; Margolin, Alexey L.</b> ; Tetrahedron Letters; <b>vol.</b> 31; nb. 47; (1990); p. 6797 - 6798, <a href="#">View in Reaxys</a>	
15 of 21	Type	[alpha]
	Solvent	neat (no solvent)

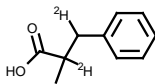
	Optical Rotatory Power [deg]	23
	Wavelength [nm]	589
	Temperature [°C]	25
	<b>Gennari, Cesare; Venturini, Isabella; Gislón, Gabriele; Schimperna, Giuliana;</b> Tetrahedron Letters; <b>vol.</b> 28; nb. 2; (1987); p. 227 - 230, <a href="#">View in Reaxys</a>	
16 of 21	Type	[alpha]
	Concentration	1.2 g/100ml
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	-29.6
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Potapov, V. M.; Dem'yanovich, V. M.; Vendrova, O. E.; Khlebnikov, V. A.;</b> Zhurnal Organicheskoi Khimii; <b>vol.</b> 18; nb. 6; (1982); p. 1205 - 1208, 1041 - 1043, <a href="#">View in Reaxys</a>	
17 of 21	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	-25.1
	Wavelength [nm]	589
	<b>Evans, D. A.; Ennis, M. D.; Mathre, D. J.;</b> Journal of the American Chemical Society; <b>vol.</b> 104; nb. 6; (1982); p. 1737 - 1739, <a href="#">View in Reaxys</a>	
18 of 21	Type	[alpha]
	Optical Rotatory Power [deg]	-23.5
	Wavelength [nm]	589
	<b>Simon, Helmut; Guenther, Helmut; Bader, Johann; Tischer, Wilhelm;</b> Angewandte Chemie; <b>vol.</b> 93; nb. 10; (1981); p. 897 - 898, <a href="#">View in Reaxys</a>	
19 of 21	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	-29.6
	Wavelength [nm]	589
	Temperature [°C]	20
	<b>Potatov, V. M.; Dem'yanovich, V. M.; Vendrova, O. E.; Strel'tsova, E. S.;</b> Journal of Organic Chemistry USSR (English Translation); <b>vol.</b> 17; nb. 11; (1981); p. 2080 - 2083; Zhurnal Organicheskoi Khimii; <b>vol.</b> 17; nb. 11; (1981); p. 2329 - 2333, <a href="#">View in Reaxys</a>	
20 of 21	Type	[alpha]
	Solvent	neat (no solvent)
	Optical Rotatory Power [deg]	-24.6
	Wavelength [nm]	589
	Temperature [°C]	22
	<b>Schrecker;</b> Journal of Organic Chemistry; <b>vol.</b> 22; (1957); p. 33, <a href="#">View in Reaxys</a>	
21 of 21	Type	[alpha]
	Concentration	c=0.025
	Solvent	ethanol

	Optical Rotatory Power [deg]	-11.5
	Wavelength [nm]	589
	Temperature [°C]	20
DeTar; Weis; Journal of the American Chemical Society; vol. 79; (1957); p. 3045,3048, <a href="#">View in Reaxys</a>		
Circular Dichroism (2)		
Solvent	Comment	References
ethanol	215 - 280 nm	Potatov, V. M.; Dem'yanovich, V. M.; Vendrova, O. E.; Strel'tsova, E. S.; Journal of Organic Chemistry USSR (English Translation); vol. 17; nb. 11; (1981); p. 2080 - 2083; Zhurnal Organicheskoi Khimii; vol. 17; nb. 11; (1981); p. 2329 - 2333, <a href="#">View in Reaxys</a>
2,2,4-trimethyl-pentane	220 - 275 nm	Potatov, V. M.; Dem'yanovich, V. M.; Vendrova, O. E.; Strel'tsova, E. S.; Journal of Organic Chemistry USSR (English Translation); vol. 17; nb. 11; (1981); p. 2080 - 2083; Zhurnal Organicheskoi Khimii; vol. 17; nb. 11; (1981); p. 2329 - 2333, <a href="#">View in Reaxys</a>
NMR Spectroscopy (15)		
1 of 15	Description	Chemical shifts
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	300
	Zupancic, Borut; Mohar, Barbara; Stephan, Michel; Organic Letters; vol. 12; nb. 13; (2010); p. 3022 - 3025, <a href="#">View in Reaxys</a>	
2 of 15	Description	Chemical shifts
	Nucleus	1H
	Solvents	CDCl3
	Frequency [MHz]	300
	Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki; Tetrahedron; vol. 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a> ; Green, Rachel; Merritt, Andrew T.; Bull, Steven D.; Chemical Communications (Cambridge, United Kingdom); nb. 4; (2008); p. 508 - 510, <a href="#">View in Reaxys</a>	
3 of 15	Description	Chemical shifts
	Nucleus	13C
	Solvents	CDCl3
	Frequency [MHz]	75.5
	Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki; Tetrahedron; vol. 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a> ; Green, Rachel; Merritt, Andrew T.; Bull, Steven D.; Chemical Communications (Cambridge, United Kingdom); nb. 4; (2008); p. 508 - 510, <a href="#">View in Reaxys</a>	
4 of 15	Description	Chemical shifts
	Nucleus	1H
	Solvents	CDCl3
	Frequency [MHz]	400
	Davies, Stephen G.; Garner, A. Christopher; Roberts, Paul M.; Smith, Andrew D.; Sweet, Miles J.; Thomson, James E.; Organic and Biomolecular Chemistry; vol. 4; nb. 14; (2006); p. 2753 - 2768, <a href="#">View in Reaxys</a>	
5 of 15	Nucleus	1H
	Coupling Nuclei	1H
	Solvents	CDCl3
	Frequency [MHz]	300
	Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki; Tetrahedron; vol. 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a>	
6 of 15	Description	Spectrum
	Nucleus	13C



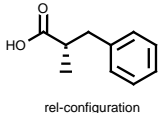
	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	50
	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Le-cumberri, Ainara; Linden, Anthony</b> ; Organic Letters; <b>vol. 3</b> ; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a>	
	Description	Spectrum
	Nucleus	<sup>1</sup> H
7 of 15	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Le-cumberri, Ainara; Linden, Anthony</b> ; Organic Letters; <b>vol. 3</b> ; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a>	
	Nucleus	<sup>1</sup> H
	Coupling Nuclei	<sup>1</sup> H
8 of 15	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Le-cumberri, Ainara; Linden, Anthony</b> ; Organic Letters; <b>vol. 3</b> ; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a>	
	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
9 of 15	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Le-cumberri, Ainara; Linden, Anthony</b> ; Organic Letters; <b>vol. 3</b> ; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a>	
	Description	Chemical shifts
	Nucleus	<sup>13</sup> C
10 of 15	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	50
	<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Le-cumberri, Ainara; Linden, Anthony</b> ; Organic Letters; <b>vol. 3</b> ; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a>	
	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
11 of 15	Coupling Nuclei	<sup>1</sup> H
	Solvents	CDCl <sub>3</sub>
	<b>Hintermann, Tobias; Seebach, Dieter</b> ; Helvetica Chimica Acta; <b>vol. 81</b> ; nb. 11; (1998); p. 2093 - 2126, <a href="#">View in Reaxys</a>	
	Description	Chemical shifts
	Nucleus	<sup>1</sup> H
12 of 15	Solvents	CDCl <sub>3</sub>
	<b>Gennari, Cesare; Schimperna, Giuliana; Venturini, Isabella</b> ; Tetrahedron; <b>vol. 44</b> ; nb. 13; (1988); p. 4221 - 4232, <a href="#">View in Reaxys</a> ; <b>Wilson, Kenneth E.; Burk, Robert M.; Biftu, Tesfaye; Ball, Richard G.; Hoogsteen, Karst</b> ; Journal of Organic Chemistry; <b>vol. 57</b> ; nb. 28; (1992); p. 7151 - 7158, <a href="#">View in Reaxys</a> ; <b>Tanner, David; Birgersson, Carin; Gogoll, Adolf; Luthman, Kristina</b> ; Tetrahedron; <b>vol. 50</b> ; nb. 32; (1994); p. 9797 - 9824, <a href="#">View in Reaxys</a> ; <b>Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John</b> ; Tetrahedron; <b>vol. 52</b> ; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a> ; <b>Myers, Andrew G.; Yang, Bryant H.; Chen, Hou; McKinstry, Lydia; Kopecky, David J.; Gleason, James L.</b> ; Journal of the American Chemical Society; <b>vol. 119</b> ; nb. 28; (1997); p. 6496 - 6511, <a href="#">View in Reaxys</a>	
	Description	Chemical shifts
	Nucleus	<sup>13</sup> C
	Solvents	CDCl <sub>3</sub>
13 of 15	Description	Chemical shifts
	Nucleus	<sup>13</sup> C
	Solvents	CDCl <sub>3</sub>

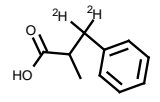
	<b>Gennari, Cesare; Schimperna, Giuliana; Venturini, Isabella; Tetrahedron; vol. 44; nb. 13; (1988); p. 4221 - 4232, <a href="#">View in Reaxys</a>; Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John; Tetrahedron; vol. 52; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a>; Myers, Andrew G.; Yang, Bryant H.; Chen, Hou; McKinstry, Lydia; Kopecky, David J.; Gleason, James L.; Journal of the American Chemical Society; vol. 119; nb. 28; (1997); p. 6496 - 6511, <a href="#">View in Reaxys</a></b>		
14 of 15	Description	Spin-spin coupling constants	
	Solvents	CDCl3	
	Comment	1H-1H	
	<b>Gennari, Cesare; Schimperna, Giuliana; Venturini, Isabella; Tetrahedron; vol. 44; nb. 13; (1988); p. 4221 - 4232, <a href="#">View in Reaxys</a>; Wilson, Kenneth E.; Burk, Robert M.; Biftu, Tesfaye; Ball, Richard G.; Hoogsteen, Karst; Journal of Organic Chemistry; vol. 57; nb. 28; (1992); p. 7151 - 7158, <a href="#">View in Reaxys</a>; Tanner, David; Birgersson, Carin; Gogoll, Adolf; Luthman, Kristina; Tetrahedron; vol. 50; nb. 32; (1994); p. 9797 - 9824, <a href="#">View in Reaxys</a>; Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John; Tetrahedron; vol. 52; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a>; Myers, Andrew G.; Yang, Bryant H.; Chen, Hou; McKinstry, Lydia; Kopecky, David J.; Gleason, James L.; Journal of the American Chemical Society; vol. 119; nb. 28; (1997); p. 6496 - 6511, <a href="#">View in Reaxys</a></b>		
15 of 15	Nucleus	1H	
	Original Text	<sup>1</sup> H NMR (CDCl <sub>3</sub> ) δ 7.33-7.19 (m, 5H), 3.10 (dd, J=13.5, 6.5, 1H), 2.83-2.74 (m, 1H), 2.79 (dd, J=13.5, 8 Hz, 1H), 1.20 (d, J=7 Hz, 3H)	
	<b>Patent; Bio-Mega/Boehringer Ingelheim Research, Inc.; US5672586; (1997); (A1) English, <a href="#">View in Reaxys</a></b>		
<b>IR Spectroscopy (5)</b>			
Description	Solvent	Comment	References
Bands	CHCl3		<b>Kotake, Tomoya; Hayashi, Yoshio; Rajesh, S.; Mukai, Yoshie; Takiguchi, Yuka; Kimura, Tooru; Kiso, Yoshiaki; Tetrahedron; vol. 61; nb. 15; (2005); p. 3819 - 3834, <a href="#">View in Reaxys</a></b>
Bands	KBr		<b>Palomo, Claudio; Oiarbide, Mikel; Mielgo, Antonia; Gonzalez, Alberto; Garcia, Jesus M.; Landa, Cristina; Lecumberri, Ainara; Linden, Anthony ; Organic Letters; vol. 3; nb. 21; (2001); p. 3249 - 3252, <a href="#">View in Reaxys</a></b>
Bands	neat (no solvent)	2976 - 1707 cm <sup>**</sup> (-1)	<b>Myers, Andrew G.; Yang, Bryant H.; Chen, Hou; McKinstry, Lydia; Kopecky, David J.; Gleason, James L.; Journal of the American Chemical Society; vol. 119; nb. 28; (1997); p. 6496 - 6511, <a href="#">View in Reaxys</a></b>
Bands	KBr	3420 - 1693 cm <sup>**</sup> (-1)	<b>Tyrrell, Elizabeth; Tsang, Michael W. H.; Skinner, George A.; Fawcett, John; Tetrahedron; vol. 52; nb. 29; (1996); p. 9841 - 9852, <a href="#">View in Reaxys</a></b>
Bands	neat (no solvent)	3400 - 700 cm <sup>**</sup> (-1)	<b>Wilson, Kenneth E.; Burk, Robert M.; Biftu, Tesfaye; Ball, Richard G.; Hoogsteen, Karst; Journal of Organic Chemistry; vol. 57; nb. 28; (1992); p. 7151 - 7158, <a href="#">View in Reaxys</a></b>

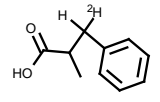
Reaxys ID 1964176 <a href="#">View in Reaxys</a>		4/15
		<b>Chemical Name:</b> 2,3-dideutero-2-methyl-3-phenylpropionic acid; 2,3-dideutero-2-methyl-3-phenylpropanoic acid; 2,3-Dideutero-2-methyl-3-phenylpropionsaeure <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>CAS Registry Number:</b> 39949-56-9; 70841-95-1 <b>Molecular Weight:</b> 166.188 <b>Linear Structure Formula:</b> C <sub>10</sub> (2)H <sub>10</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-QTQOOCSTSA-N <b>Note:</b>
<b>Substance Label (3)</b>		
Label	References	
2e	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto; Chemistry--A European Journal; vol. 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a></b>	

1b	<b>Spassov; Stefanova</b> ; Journal of Molecular Structure; <b>vol.</b> 53; (1979); p. 219,220,223, <a href="#">View in Reaxys</a>		
4a/4b	<b>Bright et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 38; (1973); p. 2554, <a href="#">View in Reaxys</a>		
<b>Related Structure (1)</b>			
References			
<b>Bright et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 38; (1973); p. 2554, <a href="#">View in Reaxys</a>			
<b>Melting Point (1)</b>			
Melting Point [°C]	References		
35 - 36	<b>Bright et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 38; (1973); p. 2554, <a href="#">View in Reaxys</a>		
<b>Boiling Point (1)</b>			
Boiling Point [°C]	Pressure [Torr]	References	
142	2	<b>Bright et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 38; (1973); p. 2554, <a href="#">View in Reaxys</a>	
<b>Conformation (1)</b>			
Object of Investigation	References		
Conformation	<b>Spassov; Stefanova</b> ; Journal of Molecular Structure; <b>vol.</b> 53; (1979); p. 219,220,223, <a href="#">View in Reaxys</a>		
<b>NMR Spectroscopy (5)</b>			
1 of 5	Description	Chemical shifts	
	Nucleus	1H	
	Solvents	CDCl3	
	Frequency [MHz]	200	
	Comment	mixture of isomers	
	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>		
2 of 5	Description	Chemical shifts	
	Nucleus	13C	
	Solvents	CDCl3	
	Frequency [MHz]	50	
	Comment	mixture of isomers	
	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>		
3 of 5	Nucleus	13C	
	Coupling Nuclei	2H	
	Solvents	CDCl3	
	Frequency [MHz]	50	
	Comment	mixture of isomers	
	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>		
4 of 5	Description	NMR	
	Comment	1H	
	<b>Spassov; Stefanova</b> ; Journal of Molecular Structure; <b>vol.</b> 53; (1979); p. 219,220,223, <a href="#">View in Reaxys</a>		
5 of 5	Description	NMR	
	<b>Bright et al.</b> ; Journal of Organic Chemistry; <b>vol.</b> 38; (1973); p. 2554, <a href="#">View in Reaxys</a>		
<b>IR Spectroscopy (1)</b>			
Description	Solvent	Comment	References
Bands	neat (no solvent)	mixture of isomers	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>
<b>Mass Spectrometry (1)</b>			

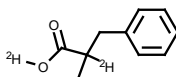
Description	References
electron impact (EI); spectrum	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>

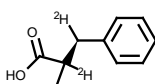
Reaxys ID 14751433 <a href="#">View in Reaxys</a>	5/15
	<b>Chemical Name:</b> 2-methyl-3-phenylpropionic acid <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>Molecular Weight:</b> 164.204 <b>Linear Structure Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>InChIKey:</b> MCIIDRLDHRQKPH-QMMMGPBSA-N <b>Note:</b>

Reaxys ID 2453211 <a href="#">View in Reaxys</a>	6/15
	<b>Chemical Name:</b> 2-methyl-3-phenylpropionic-3,3-d2 acid <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>Molecular Weight:</b> 166.188 <b>Linear Structure Formula:</b> C <sub>10</sub> H <sub>10</sub> D <sub>2</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-RJSZUWSASA-N <b>Note:</b>
<b>Boiling Point (1)</b>	
Boiling Point [°C]	Pressure [Torr]
113 - 118	0.6 - 0.9
References	
<b>Nibbering; de Boer</b> ; Organic Mass Spectrometry; <b>vol.</b> 2; (1969); p. 157,161,164,169,173, <a href="#">View in Reaxys</a>	

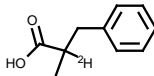
Reaxys ID 4411595 <a href="#">View in Reaxys</a>	7/15
	<b>Chemical Name:</b> 3-deuterio-2-methyl-3-phenylpropionic acid; 2-methyl-3-phenylpropionic-3-d acid <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>CAS Registry Number:</b> 87482-91-5 <b>Molecular Weight:</b> 165.196 <b>Linear Structure Formula:</b> C <sub>10</sub> ( <sup>2</sup> H)H <sub>11</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-WHRKIXHSSA-N <b>Note:</b>
<b>Substance Label (1)</b>	
Label	References
13e	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>
<b>NMR Spectroscopy (4)</b>	
1 of 4	Description
	Chemical shifts
	Nucleus
	Solvents
	Frequency [MHz]
	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>
2 of 4	Nucleus
	Coupling Nuclei

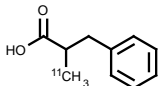
3 of 4	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	200
	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>	
	Description	Chemical shifts
	Nucleus	<sup>13</sup> C
4 of 4	Solvents	CDCl <sub>3</sub>
	Frequency [MHz]	50
	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>	
	Nucleus	<sup>13</sup> C
	Coupling Nuclei	<sup>2</sup> H
<b>IR Spectroscopy (1)</b>		
Description	Solvent	References
Bands	neat (no solvent)	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>
<b>Mass Spectrometry (1)</b>		
Description	References	
electron impact (EI); spectrum	<b>Concellon, Jose M.; Rodriguez-Solla, Humberto</b> ; Chemistry--A European Journal; <b>vol.</b> 8; nb. 19; (2002); p. 4493 - 4497, <a href="#">View in Reaxys</a>	

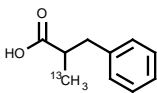
Reaxys ID 2581326 <a href="#">View in Reaxys</a>		8/15
		<b>Chemical Name:</b> 2-Methyl-3-phenylpropionsaeure-2d <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>Molecular Weight:</b> 166.188 <b>Linear Structure Formula:</b> C <sub>10</sub> H <sub>10</sub> D <sub>2</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-FMSOFXHYSAN <b>Note:</b>
<b>Boiling Point (1)</b>		
Boiling Point [°C]	Pressure [Torr]	References
106 - 107	3	<b>Melander; Bergman</b> ; Acta Chemica Scandinavica (1947-1973); <b>vol.</b> 25; (1971); p. 2264,2265, <a href="#">View in Reaxys</a>
<b>NMR Spectroscopy (1)</b>		
1 of 1	Description	NMR
	Comment	<sup>1</sup> H
	<b>Melander; Bergman</b> ; Acta Chemica Scandinavica (1947-1973); <b>vol.</b> 25; (1971); p. 2264,2265, <a href="#">View in Reaxys</a>	

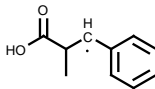
Reaxys ID 3950892 <a href="#">View in Reaxys</a>		9/15
		<b>Chemical Name:</b> (αR,βR)-α-Methyl-<α,β- <sup>2</sup> H>-dihydrozimtat; (αR,βR)-α-Methyl-[α,β- <sup>2</sup> H]-dihydrozimtat <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>CAS Registry Number:</b> 39949-56-9; 70841-95-1

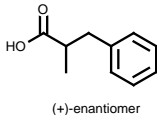
			<b>Molecular Weight:</b> 166.188 <b>Linear Structure Formula:</b> C <sub>10</sub> H <sub>10</sub> D <sub>2</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-LLYNPMAHSA-N <b>Note:</b>
<b>Substance Label (1)</b>			
Label		References	
5c		<b>Hashimoto et al.</b> ; Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie; <b>vol.</b> 356; (1975); p. 1203,1208, <a href="#">View in Reaxys</a>	
<b>Optical Rotatory Power (1)</b>			
1 of 1	Type	[alpha]	
	Optical Rotatory Power [deg]	-20.5	
	Wavelength [nm]	589	
	<b>Hashimoto et al.</b> ; Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie; <b>vol.</b> 356; (1975); p. 1203,1208, <a href="#">View in Reaxys</a>		

Reaxys ID 4135393 <a href="#">View in Reaxys</a>		10/15	
		<b>Chemical Name:</b> (+)-2-Deuterio-2-methyl-3-phenyl-propan-saeure <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>CAS Registry Number:</b> 34916-95-5; 34916-96-6; 34916-98-8 <b>Molecular Weight:</b> 165.196 <b>Linear Structure Formula:</b> C <sub>10</sub> H <sub>11</sub> DO <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-BNEYPBHNSA-N <b>Note:</b>	
<b>Boiling Point (1)</b>			
Boiling Point [°C]	Pressure [Torr]	References	
120	1.2	<b>Cram,D.J.; Wingrove,A.S.</b> ; Journal of the American Chemical Society; <b>vol.</b> 86; (1964); p. 5490 - 5496, <a href="#">View in Reaxys</a>	
<b>Refractive Index (1)</b>			
Refractive Index	Wavelength [nm]	Temperature [°C]	References
1.5112	589	25	<b>Cram,D.J.; Wingrove,A.S.</b> ; Journal of the American Chemical Society; <b>vol.</b> 86; (1964); p. 5490 - 5496, <a href="#">View in Reaxys</a>

Reaxys ID 4311692 <a href="#">View in Reaxys</a>		11/15
		<b>Chemical Name:</b> 2-benzyl-<3-11C>propionic acid; 2-benzyl-[3-11C]propionic acid <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>CAS Registry Number:</b> 135154-83-5 <b>Molecular Weight:</b> 163.193 <b>Linear Structure Formula:</b> C <sub>9</sub> ( <sup>11</sup> )CH <sub>12</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-BJUDXGMSA-N <b>Note:</b>
<b>Substance Label (1)</b>		
Label	References	
2	<b>Gee, Antony; Langstroem, Bengt;</b> Acta Chemica Scandinavica; <b>vol.</b> 45; nb. 4; (1991); p. 431 - 435, <a href="#">View in Reaxys</a>	

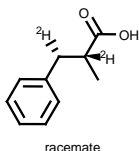
Reaxys ID 4311700 <a href="#">View in Reaxys</a>	12/15
	<b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>Molecular Weight:</b> 165.193 <b>Linear Structure Formula:</b> C <sub>9</sub> ( <sup>13</sup> )CH <sub>12</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-OUBTZVSYSA-N <b>Note:</b>

Reaxys ID 5932621 <a href="#">View in Reaxys</a>		13/15
		<b>Molecular Formula:</b> C <sub>10</sub> H <sub>11</sub> O <sub>2</sub> <b>CAS Registry Number:</b> 109686-81-9; 109686-84-2; 111865-91-9 <b>Molecular Weight:</b> 163.196 <b>Linear Structure Formula:</b> C <sub>10</sub> H <sub>11</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> GFQLUJVNIPCXS-FUHFFFAOYSA-N <b>Note:</b>
<b>Substance Label (1)</b>		
Label	References	
6	<b>Gilbert, Bruce C.; Scarratt, Cathryn J.; Thomas, C. Barry; Young, John;</b> Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1987); p. 371 - 380, <a href="#">View in Reaxys</a>	
<b>ESR Spectroscopy (3)</b>		
Description	Comment	References
ESR-hyperfine coupling constants	1H.	<b>Gilbert, Bruce C.; Scarratt, Cathryn J.; Thomas, C. Barry; Young, John;</b> Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1987); p. 371 - 380, <a href="#">View in Reaxys</a>
Signals		<b>Gilbert, Bruce C.; Scarratt, Cathryn J.; Thomas, C. Barry; Young, John;</b> Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1987); p. 371 - 380, <a href="#">View in Reaxys</a>
g-factor		<b>Gilbert, Bruce C.; Scarratt, Cathryn J.; Thomas, C. Barry; Young, John;</b> Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1987); p. 371 - 380, <a href="#">View in Reaxys</a>

Reaxys ID 6131336 <a href="#">View in Reaxys</a>		14/15
<div></div>		<b>Chemical Name:</b> (+)-β-Phenylisobutyrsaeure <b>Molecular Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>Molecular Weight:</b> 164.204 <b>Linear Structure Formula:</b> C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> <b>Type of Substance:</b> isocyclic <b>InChIKey:</b> MCIIDRLDHRQKPH-UHFFFAOYSA-N <b>Note:</b>
<b>Substance Label (1)</b>		
Label	References	
(+)	<b>Kashiwagi, T. et al.;</b> Tetrahedron; <b>vol.</b> 26; (1970); p. 3619 - 3629, <a href="#">View in Reaxys</a>	
<b>Purification (1)</b>		
Purification (method)	References	
quinine	<b>Kashiwagi, T. et al.;</b> Tetrahedron; <b>vol.</b> 26; (1970); p. 3619 - 3629, <a href="#">View in Reaxys</a>	
<b>Optical Rotatory Power (1)</b>		
1 of 1	Type	[alpha]
	Concentration	9.7 g/100ml



Solvent	ethanol
Optical Rotatory Power [deg]	22.2
Wavelength [nm]	589
Temperature [°C]	13
<b>Kashiwagi, T. et al.</b> ; Tetrahedron; <b>vol.</b> 26; (1970); p. 3619 - 3629, <a href="#">View in Reaxys</a>	

Reaxys ID 8139855 <a href="#">View in Reaxys</a>	15/15
 <p>racemate</p>	<p><b>Molecular Formula:</b> C<sub>10</sub>H<sub>12</sub>O<sub>2</sub></p> <p><b>Molecular Weight:</b> 166.188</p> <p><b>Linear Structure Formula:</b> C<sub>10</sub>H<sub>10</sub>D<sub>2</sub>O<sub>2</sub></p> <p><b>Type of Substance:</b> isocyclic</p> <p><b>InChIKey:</b> MCIIDRLDHRQKPH-GYRIUEEPSA-N</p> <p><b>Note:</b></p>