

Maltol

Other names:	4H-Pyran-4-one, 3-hydroxy-2-methyl- Larixic acid Larixinic acid Palatone 3-Hydroxy-2-methyl-4-pyrone 3-Hydroxy-2-methylpyrone 3-Hydroxy-2-methyl-4-pyranone 3-Hydroxy-2-methyl-1,4-pyrone Corps praline Talmon Vetol 2-Methyl pyromeconic acid 2-Methyl-3-hydroxy-4-pyrone 3-Hydroxy-2-methyl-«gamma»-pyrone 3-Hydroxy-2-methyl-4H-pyran-4-one 2-Methyl-3-oxy-«gamma»-pyrone Veltol 2-Methyl-3-hydroxy-4-pyranone 3-hydroxy-2-methylpyran-4-one 5-Hydroxy-6-methyl-4H-pyran-4-one NSC 2829 5-Hydroxy-6-methyl-4H-pyran-4-one (maltol) 3-Hydroxy-2-methyl-4(4H)-pyranone 3-Hydroxy-2-methyl-4-pyrone(maltol) 3-Hydroxy-2-methyl-4H-pyranone 3-Hydroxy-2-methyl-4H-pyran-4-one (maltol) 2-methyl-3-hydroxy-4-pyranone (maltol) 2-hydroxy-3-methyl-4H-pyran-4-one (maltol) 3-Hydroxy-2-pyran-4-one (maltol)
Inchi:	InChI=1S/C6H6O3/c1-4-6(8)5(7)2-3-9-4/h2-3,8H,1H3
InchiKey:	XPCTZQVDEJYUGT-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	Cc1occc(=O)c1O
Mol. weight [g/mol]:	126.11
CAS:	118-71-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	0.654		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpol	1092.20		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1110.80		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1110.80		NIST Webbook

ripol	1110.00	NIST Webbook
ripol	1092.20	NIST Webbook
ripol	1133.00	NIST Webbook
ripol	1130.00	NIST Webbook
ripol	1091.00	NIST Webbook
ripol	1963.00	NIST Webbook
ripol	1943.00	NIST Webbook
ripol	2002.00	NIST Webbook
ripol	2012.00	NIST Webbook
ripol	1991.00	NIST Webbook
ripol	1943.00	NIST Webbook
ripol	1949.00	NIST Webbook
ripol	1996.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1978.00	NIST Webbook
ripol	1969.00	NIST Webbook
ripol	1968.00	NIST Webbook
ripol	1968.00	NIST Webbook
ripol	1975.00	NIST Webbook
ripol	2000.00	NIST Webbook
ripol	1995.00	NIST Webbook
ripol	2000.00	NIST Webbook
ripol	1998.00	NIST Webbook
ripol	2003.00	NIST Webbook
ripol	2004.00	NIST Webbook
ripol	1954.00	NIST Webbook
ripol	2004.00	NIST Webbook
ripol	2006.00	NIST Webbook
ripol	1964.00	NIST Webbook
ripol	1977.00	NIST Webbook
ripol	1936.00	NIST Webbook
ripol	1936.00	NIST Webbook
ripol	1980.00	NIST Webbook
ripol	1981.00	NIST Webbook
ripol	1985.00	NIST Webbook
ripol	1974.00	NIST Webbook
ripol	2003.00	NIST Webbook
ripol	2004.00	NIST Webbook
ripol	1998.00	NIST Webbook
ripol	1954.00	NIST Webbook
ripol	1954.00	NIST Webbook
ripol	1960.00	NIST Webbook
ripol	1980.00	NIST Webbook
ripol	1981.00	NIST Webbook

ripol	1960.00	NIST Webbook
ripol	1954.00	NIST Webbook
ripol	1961.00	NIST Webbook
ripol	1973.00	NIST Webbook
ripol	1961.00	NIST Webbook
ripol	1938.00	NIST Webbook
ripol	1947.00	NIST Webbook
ripol	1965.00	NIST Webbook
ripol	1959.00	NIST Webbook
ripol	1988.00	NIST Webbook
ripol	1968.00	NIST Webbook
ripol	1958.00	NIST Webbook
ripol	1961.00	NIST Webbook
ripol	1925.00	NIST Webbook
ripol	1975.00	NIST Webbook
ripol	1967.00	NIST Webbook
ripol	1965.00	NIST Webbook
ripol	1975.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118718&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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