

2-Furanmethanol, 5-methyl-

Other names:	5-Methyl-2-furfuryl alcohol (5-Methylfur-2-yl)-methanol 5-methylfurfuryl alcohol 5-methyl-2-furanmethanol (5-methylfurfur-2-yl)-methanol
Inchi:	InChI=1S/C6H8O2/c1-5-2-3-6(4-7)8-5/h2-3,7H,4H2,1H3
InchiKey:	VOZFDEJGHQWZHU-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	Cc1ccc(CO)o1
Mol. weight [g/mol]:	112.13
CAS:	3857-25-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.82		Crippen Method
logp	1.080		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
rinpol	958.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1727.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1727.00		NIST Webbook

ripol	1678.00	NIST Webbook
ripol	1677.00	NIST Webbook
ripol	1713.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C3857258&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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