2-Furanmethanethiol, 5-methyl-

Other names:	(5-Methyl-2-furyl)methanethiol
	2-Methyl-5-thiomethylfuran
	5-Methyl-2-furfurylmercaptan
	5-Methyl-2-furfurylthiol
	5-Methylfurfuryl mercaptan
Inchi:	InChI=1S/C6H8OS/c1-5-2-3-6(4-8)7-5/h2-3,8H,4H2,1H3
InchiKey:	MGLMZOFGBDYNMH-UHFFFAOYSA-N
Formula:	C6H8OS
SMILES:	Cc1ccc(CS)o1
Mol. weight [g/mol]:	128.19
CAS:	59303-05-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.63		Crippen Method
logp	2.018		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
rinpol	995.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	993.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1473.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1497.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59303058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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