2-Furylmethylsulfide

Other names:	Methyl furfuryl sulfide
	2-Methylsulfanyl-furan
	Furan,2-(methylthio)-
Inchi:	InChI=1S/C5H6OS/c1-7-5-3-2-4-6-5/h2-4H,1H3
InchiKey:	QNQUVXCNWQTHHY-UHFFFAOYSA-N
Formula:	C5H6OS
SMILES:	CSc1ccco1
Mol. weight [g/mol]:	114.17
CAS:	13129-38-9

Physical Properties

Property code	Value	Unit	Source
ie	8.58 ± 0.05	eV	NIST Webbook
log10ws	-5.95		Crippen Method
logp	2.002		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
rinpol	902.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	865.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1492.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13129389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
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