2-Furanthiol

Other names: furan-2-thiol
Inchi: InChI=1S/C4H4OS/c6-4-2-1-3-5-4/h1-3,6H
InchiKey: CMDKYFGIJALPLS-UHFFFAOYSA-N
Formula: C4H4OS
SMILES: Sc1ccco1
Mol. weight [g/mol]: 100.14
CAS: 13129-35-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	1.568		Crippen Method
mcvol	69.980	ml/mol	McGowan Method
rinpol	912.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	914.00		NIST Webbook
ripol	1443.00		NIST Webbook
ripol	1443.00		NIST Webbook

Sources

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=C13129356&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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