2,5-Dimethyl-3-furanthiol

Other names: 2,5-dimethylfuran-3-thiol
3-Furanthiol, 2,5-dimethyl-
Inchi: InChI=1S/C6H8OS/c1-4-3-6(8)5(2)7-4/h3,8H,1-2H3
InchiKey: DBBHCZMXKBCICL-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: Cc1cc(S)c(C)o1
Mol. weight [g/mol]: 128.19
CAS: 55764-23-3

Physical Properties

Property code	Value	Unit	Source
ie	8.23 ± 0.05	eV	NIST Webbook
log10ws	-6.67		Crippen Method
logp	2.185		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	968.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55764233&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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