

2-Thiophenethiol

Other names:	2-Mercaptothiophene Thiophene-2-thiol 2-thienylthiol 2-Thienyl mercaptan «alpha»-Thienyl mercaptan
Inchi:	InChI=1S/C4H4S2/c5-4-2-1-3-6-4/h1-3,5H
InchiKey:	SWEDAZLCYJDAGW-UHFFFAOYSA-N
Formula:	C4H4S2
SMILES:	Sc1cccs1
Mol. weight [g/mol]:	116.20
CAS:	7774-74-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.74		Crippen Method
logp	2.037		Crippen Method
mcvol	80.460	ml/mol	McGowan Method
rinpol	946.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	976.70		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	961.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1530.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7774745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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