

2-Thiophenemethanethiol

Other names:	Thenyl mercaptan 2-Thienylmethanethiol 2-Thenyl mercaptan Thiophene-2-methanethiol 2-Thiophenemethenethiol
Inchi:	InChI=1S/C5H6S2/c6-4-5-2-1-3-7-5/h1-3,6H,4H2
InchiKey:	GCZQHDFWKVMZOE-UHFFFAOYSA-N
Formula:	C5H6S2
SMILES:	SCc1cccs1
Mol. weight [g/mol]:	130.23
CAS:	6258-63-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	2.178		Crippen Method
mcvol	94.550	ml/mol	McGowan Method
ripol	1107.00		NIST Webbook
ripol	1105.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1702.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6258635&Units=SI

Legend

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

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