

Thiophene, 2-ethylthio

Other names: 2-(ethylsulfanyl)thiophene
Inchi: InChI=1S/C6H8S2/c1-2-7-6-4-3-5-8-6/h3-5H,2H2,1H3
InchiKey: XLEZAQDRMZZJTO-UHFFFAOYSA-N
Formula: C6H8S2
SMILES: CCSc1cccs1
Mol. weight [g/mol]: 144.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	2.860		Crippen Method
mcvol	108.640	ml/mol	McGowan Method
rinpol	1106.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1106.00		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=R57747&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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