Thiophene, 3-ethylthio

Inchi: InChI=1S/C6H8S2/c1-2-8-6-3-4-7-5-6/h3-5H,2H2,1H3
InchiKey: UBWDXOWKUVMGNS-UHFFFAOYSA-N
Formula: C6H8S2
SMILES: CCSc1ccsc1
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	1141.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1152.00		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=R57797&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

Latest version available from:

https://www.chemeo.com/cid/20-574-2/Thiophene-3-ethylthio.pdf

Generated by Cheméo on 2024-10-12 08:01:24.171005249 +0000 UTC m=+3300946.807974497.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.