

Thieno[2,3-b]thiophene, 2-ethyl-

Other names: 5-ethylthieno[2,3-d]thiophene
Inchi: InChI=1S/C8H8S2/c1-2-7-5-6-3-4-9-8(6)10-7/h3-5H,2H2,1H3
InchiKey: WZCVGJWDRWSKOR-UHFFFAOYSA-N
Formula: C8H8S2
SMILES: CCc1cc2ccsc2s1
Mol. weight [g/mol]: 168.28
CAS: 5912-01-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	3.525		Crippen Method
mcvol	121.660	ml/mol	McGowan Method
rinpol	1353.00		NIST Webbook
rinpol	1353.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5912016&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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