

Thiophene, 2,3-dichloro-

Other names: 2,3-Dichlorothiophene
Inchi: InChI=1S/C4H2Cl2S/c5-3-1-2-7-4(3)6/h1-2H
InchiKey: LVNVLQIXMBTMPH-UHFFFAOYSA-N
Formula: C4H2Cl2S
SMILES: Clc1ccsc1Cl
Mol. weight [g/mol]: 153.03
CAS: 17249-79-5

Physical Properties

Property code	Value	Unit	Source
ie	8.77	eV	NIST Webbook
log10ws	-2.60		Crippen Method
logp	3.055		Crippen Method
mcvol	88.590	ml/mol	McGowan Method
rinsol	1044.00		NIST Webbook
tb	446.70	K	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17249795&Units=SI>
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>

Legend

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

tb: Normal Boiling Point Temperature

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