

Thiophene, 2,5-dichloro-3-nitro-

Inchi: InChI=1S/C4HCl2NO2S/c5-3-1-2(7(8)9)4(6)10-3/h1H
InchiKey: BFQBMQKCYWOSEN-UHFFFAOYSA-N
Formula: C4HCl2NO2S
SMILES: O=[N+](O-)c1cc(Cl)sc1Cl
Mol. weight [g/mol]: 198.03
CAS: 37105-12-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	2.963		Crippen Method
mcvol	106.010	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C37105127&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

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/46-568-1/Thiophene-2-5-dichloro-3-nitro.pdf>

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