

Thiophene, 2,5-dichloro-3,4-dinitro-

Other names:	2,5-Dichloro-3,4-dinitrothiophene
Inchi:	InChI=1S/C4Cl2N2O4S/c5-3-1(7(9)10)2(8(11)12)4(6)13-3
InchiKey:	UNRSLHGBQKYYSF-UHFFFAOYSA-N
Formula:	C4Cl2N2O4S
SMILES:	O=[N+]([O-])c1c(Cl)sc(Cl)c1[N+](=O)[O-]
Mol. weight [g/mol]:	243.03
CAS:	51584-21-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	2.871		Crippen Method
mcvol	123.430	ml/mol	McGowan Method

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=C51584215&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

Latest version available from:

<https://www.chemeo.com/cid/77-679-4/Thiophene-2-5-dichloro-3-4-dinitro.pdf>

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