Thiophene, 2-chloro-3,5-dinitro-

Inchi:	InChI=1S/C4HClN2O4S/c5-4-2(6(8)9)1-3(12-4)7(10)11/h1H
InchiKey:	APWYALWJANASTQ-UHFFFAOYSA-N
Formula:	C4HClN2O4S
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(Cl)s1
Mol. weight [g/mol]:	208.58
CAS:	6286-32-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	2.218		Crippen Method
mcvol	111.190	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6286324&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

Latest version available from:
https://www.chemeo.com/cid/77-704-5/Thiophene-2-chloro-3-5-dinitro.pdf
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