

Thiophene, 2-amino-3,5-dinitro-

Other names:	2,5-dinitrothiophen-2-amine
Inchi:	InChI=1S/C4H3N3O4S/c5-4-2(6(8)9)1-3(12-4)7(10)11/h1H,5H2
InchiKey:	DZRZHFOFVWAKGT-UHFFFAOYSA-N
Formula:	C4H3N3O4S
SMILES:	<chem>Nc1sc([N+](=O)[O-])cc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	189.15
CAS:	2045-70-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	1.147		Crippen Method
mcvol	108.930	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2045707&Units=SI

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/113-391-2/Thiophene-2-amino-3-5-dinitro.pdf>

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