

# 2-Thiophenine, 3,5-dinitro-n-phenyl thiophene, 2-anilino-3,5-dinitro-

Inchi:	InChI=1S/C10H7N3O4S/c14-12(15)8-6-9(13(16)17)18-10(8)11-7-4-2-1-3-5-7/h1-6,11H
InchiKey:	XTHINSIFAJZOSG-UHFFFAOYSA-N
Formula:	C10H7N3O4S
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(Nc2ccccc2)s1
Mol. weight [g/mol]:	265.25
CAS:	959-38-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.308		Crippen Method
mcvol	169.710	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C959386&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C959386&amp;Units=SI</a>

## Legend

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

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