

2,4-Dinitrothiophene

Other names:	Thiophene, 2,4-dinitro-
Inchi:	InChI=1S/C4H2N2O4S/c7-5(8)3-1-4(6(9)10)11-2-3/h1-2H
InchiKey:	RZKBGZBDWAUWMC-UHFFFAOYSA-N
Formula:	C4H2N2O4S
SMILES:	O=[N+]([O-])c1csc([N+](=O)[O-])c1
Mol. weight [g/mol]:	174.13
CAS:	5347-12-6

Physical Properties

Property code	Value	Unit	Source
ie	10.33	eV	NIST Webbook
log10ws	-2.53		Crippen Method
logp	1.564		Crippen Method
mvol	98.950	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	59.70	kJ/mol	455.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.72922e+01
Coeff. B	-7.17509e+03
Temperature range (K), min.	388.00
Temperature range (K), max.	598.89

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=C5347126&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure

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