

3-Chlorothiophene

Other names:	Thiophene, 3-chloro-
Inchi:	InChI=1S/C4H3ClS/c5-4-1-2-6-3-4/h1-3H
InchiKey:	QUBJDMPBDURTJT-UHFFFAOYSA-N
Formula:	C4H3ClS
SMILES:	Clc1ccsc1
Mol. weight [g/mol]:	118.58
CAS:	17249-80-8

Physical Properties

Property code	Value	Unit	Source
ie	8.92	eV	NIST Webbook
log10ws	-1.91		Crippen Method
logp	2.401		Crippen Method
mcpvol	76.350	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	9.39	kJ/mol	156.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17249808&Units=SI
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

Legend

hfust:	Enthalpy of fusion 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

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