3-Chlorophenyl isothiocyanate

Other names: Benzene, 1-chloro-3-isothiocyanato-
Isothiocyanic acid, 3-chlorophenyl ester
Isothiocyanic acid, m-chlorophenyl ester
Inchi: InChI=1S/C7H4ClNS/c8-6-2-1-3-7(4-6)9-5-10/h1-4H
InchiKey: WGXCKFMVBAOIFH-UHFFFAOYSA-N
Formula: C7H4ClNS
SMILES: S=C=Nc1cccc(Cl)c1
Mol. weight [g/mol]: 169.63
CAS: 2392-68-9

Physical Properties

Property code	Value	Unit	Source
hf	305.58	kJ/mol	Joback Method
hvap	48.94	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	3.074		Crippen Method
mcvol	115.700	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	574.60	K	Joback Method
tc	845.67	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2392689&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature