

Benzene, 4-chloro-1-isothiocyanato-2-methyl-

Other names:	3-chloro-6-isothiocyanatotoluene
Inchi:	InChI=1S/C8H6ClNS/c1-6-4-7(9)2-3-8(6)10-5-11/h2-4H,1H3
InchiKey:	XYTLRVPBHRTMS-UHFFFAOYSA-N
Formula:	C8H6ClNS
SMILES:	<chem>Cc1cc(Cl)ccc1N=C=S</chem>
Mol. weight [g/mol]:	183.66
CAS:	23165-53-9

Physical Properties

Property code	Value	Unit	Source
hf	273.47	kJ/mol	Joback Method
hvap	51.83	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.383		Crippen Method
mcvol	129.790	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	602.46	K	Joback Method
tc	868.07	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=C23165539&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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