

4-Chloro-2-methylphenyl isothiocyanate

Other names:	3-chloro-6-isothiocyanatotoluene
Inchi:	InChI=1S/C8H6CINS/c1-6-4-7(9)2-3-8(6)10-5-11/h2-4H,1H3
InchiKey:	XYTLRVPBHRTMS-UHFFFAOYSA-N
Formula:	C8H6CINS
SMILES:	<chem>Cc1cc(Cl)ccc1N=C=S</chem>
Mol. weight [g/mol]:	183.66

Physical Properties

Property code	Value	Unit	Source
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-4.21		Cheméo Relay (1.0)
logp	3.383		Crippen Method
mcvol	129.790	ml/mol	McGowan Method
tb	493.24	K	Cheméo Relay (1.0)
tf	296.67	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23165539&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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