4-Chloro-2-methylphenyl isothiocyanate

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: XTYLRVPBHHRTMS-UHFFFAOYSA-N
Formula: C8H6ClNS
SMILES: Cc1cc(Cl)ccc1N=C=S
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/ci990307l
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