4-Chloro-2-methylphenyl isocyanate

Other names: 4-Chloro-2-methylphenyl isocyanate
Inchi: InChI=1S/C8H6ClNO/c1-6-4-7(9)2-3-8(6)10-5-11/h2-4H,1H3
InchiKey: FTZJLXIATZSKIL-UHFFFAOYSA-N
Formula: C8H6ClNO
SMILES: Cc1cc(Cl)ccc1N=C=O
Mol. weight [g/mol]: 167.60

Physical Properties

Property code	Value	Unit	Source
hf	-56.64	kJ/mol	Cheméo Relay (1.0)
hvap	54.10	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	-3.12		Cheméo Relay (1.0)
logp	2.616		Crippen Method
mcvol	119.310	ml/mol	McGowan Method
tb	478.77	K	Cheméo Relay (1.0)
tf	293.27	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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=C37408187&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
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