3-Chloro-4-methylphenylisocyanate

Inchi: InChI=1S/C8H6ClNO/c1-6-2-3-7(10-5-11)4-8(6)9/h2-4H,1H3
InchiKey: UKTKKMZDESVUEE-UHFFFAOYSA-N
Formula: C8H6ClNO
SMILES: Cc1ccc(N=C=O)cc1Cl
Mol. weight [g/mol]: 167.59
CAS: 51488-20-1

Physical Properties

Property code	Value	Unit	Source
chl	-3900.00 ± 24.00	kJ/mol	NIST Webbook
hf	-77.00 ± 25.00	kJ/mol	NIST Webbook
hfl	-126.00 ± 24.00	kJ/mol	NIST Webbook
hvap	50.92	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	2.616		Crippen Method
mcvol	119.310	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	523.18	K	Joback Method
tc	752.02	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51488201&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

chl: Standard liquid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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