N-methyl-m-chlorobenzylamine

Other names: 3-chloro-N-methylbenzylamine
Inchi: InChI=1S/C8H10ClN/c1-10-6-7-3-2-4-8(9)5-7/h2-5,10H,6H2,1H3
InchiKey: ZPNLAQVYPIAHTO-UHFFFAOYSA-N
Formula: C8H10ClN
SMILES: CNCc1cccc(Cl)c1
Mol. weight [g/mol]: 155.62
CAS: 39191-07-6

Physical Properties

Property code	Value	Unit	Source
gf	196.72	kJ/mol	Joback Method
hf	54.34	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	47.16	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.059		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	501.70	K	Joback Method
tc	721.21	K	Joback Method
tf	301.44	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.35	J/mol×K	501.70	Joback Method
cpg	256.45	J/mol×K	538.29	Joback Method
cpg	267.80	J/mol×K	574.87	Joback Method
cpg	278.45	J/mol×K	611.46	Joback Method
cpg	288.41	J/mol×K	648.04	Joback Method
cpg	297.73	J/mol×K	684.63	Joback Method
cpg	306.43	J/mol×K	721.21	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=C39191076&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume