3,5-Dichlorobenzylamine

Inchi: InChI=1S/C7H7Cl2N/c8-6-1-5(4-10)2-7(9)3-6/h1-3H,4,10H2
InchiKey: ICIJWOWQUHHETJ-UHFFFAOYSA-N
Formula: C7H7Cl2N
SMILES: NCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 176.04
CAS: 39989-43-0

Physical Properties

Property code	Value	Unit	Source
gf	143.80	kJ/mol	Joback Method
hf	28.09	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	54.19	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.452		Crippen Method
mcvol	120.190	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	543.59	K	Joback Method
tc	783.56	K	Joback Method
tf	363.21	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.87	J/mol×K	543.59	Joback Method
cpg	242.40	J/mol×K	583.58	Joback Method
cpg	251.28	J/mol×K	623.58	Joback Method
cpg	259.54	J/mol×K	663.57	Joback Method
cpg	267.20	J/mol×K	703.57	Joback Method
cpg	274.29	J/mol×K	743.56	Joback Method
cpg	280.86	J/mol×K	783.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39989430&Units=SI

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