N-methyl-2,4-dichlorobenzylamine

Inchi: InChI=1S/C8H9Cl2N/c1-11-5-6-2-3-7(9)4-8(6)10/h2-4,11H,5H2,1H3
InchiKey: GUJXWKXDISDARD-UHFFFAOYSA-N
Formula: C8H9Cl2N
SMILES: CNCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 190.07
CAS: 5013-77-4

Physical Properties

Property code	Value	Unit	Source
gf	175.16	kJ/mol	Joback Method
hf	27.13	kJ/mol	Joback Method
hfus	23.23	kJ/mol	Joback Method
hvap	52.21	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.713		Crippen Method
mcvol	134.280	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	544.11	K	Joback Method
tc	769.70	K	Joback Method
tf	343.88	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.07	J/mol×K	544.11	Joback Method
cpg	279.03	J/mol×K	581.71	Joback Method
cpg	289.30	J/mol×K	619.31	Joback Method
cpg	298.92	J/mol×K	656.90	Joback Method
cpg	307.90	J/mol×K	694.50	Joback Method
cpg	316.27	J/mol×K	732.10	Joback Method
cpg	324.06	J/mol×K	769.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5013774&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

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