Benzenemethanamine, 3-chloro-

Other names: m-Chlorobenzylamine
3-Chlorobenzylamine
Inchi: InChI=1S/C7H8ClN/c8-7-3-1-2-6(4-7)5-9/h1-4H,5,9H2
InchiKey: BJFPYGGTDAYECS-UHFFFAOYSA-N
Formula: C7H8ClN
SMILES: NCc1cccc(Cl)c1
Mol. weight [g/mol]: 141.60
CAS: 4152-90-3

Physical Properties

Property code	Value	Unit	Source
gf	165.36	kJ/mol	Joback Method
hf	55.30	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	49.14	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.799		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	501.18	K	Joback Method
tc	735.06	K	Joback Method
tf	320.77	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.53	J/mol×K	501.18	Joback Method
cpg	222.20	J/mol×K	540.16	Joback Method
cpg	232.15	J/mol×K	579.14	Joback Method
cpg	241.43	J/mol×K	618.12	Joback Method
cpg	250.05	J/mol×K	657.10	Joback Method
cpg	258.06	J/mol×K	696.08	Joback Method
cpg	265.49	J/mol×K	735.06	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.20	K	2.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4152903&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume