Aniline, N-(3-chloropropyl)-N-methyl-

Inchi: InChI=1S/C10H14ClN/c1-12(9-5-8-11)10-6-3-2-4-7-10/h2-4,6-7H,5,8-9H2,1H3
InchiKey: GRIGFDIUVHVQCZ-UHFFFAOYSA-N
Formula: C10H14ClN
SMILES: CN(CCCCl)c1ccccc1
Mol. weight [g/mol]: 183.68

Physical Properties

Property code	Value	Unit	Source
gf	244.58	kJ/mol	Joback Method
hf	38.59	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	46.56	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.752		Crippen Method
mcvol	150.220	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1539.00		NIST Webbook
tb	504.75	K	Joback Method
tc	712.36	K	Joback Method
tf	291.27	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.42	J/mol×K	504.75	Joback Method
cpg	333.58	J/mol×K	539.35	Joback Method
cpg	347.79	J/mol×K	573.95	Joback Method
cpg	361.11	J/mol×K	608.55	Joback Method
cpg	373.57	J/mol×K	643.15	Joback Method
cpg	385.22	J/mol×K	677.75	Joback Method
cpg	396.11	J/mol×K	712.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380568&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume