2-(3-Chlorophenyl)ethylamine

Inchi: InChI=1S/C8H10ClN/c9-8-3-1-2-7(6-8)4-5-10/h1-3,6H,4-5,10H2
InchiKey: NRHVNPYOTNGECT-UHFFFAOYSA-N
Formula: C8H10ClN
SMILES: NCCc1cccc(Cl)c1
Mol. weight [g/mol]: 155.62
CAS: 13078-79-0

Physical Properties

Property code	Value	Unit	Source
gf	173.78	kJ/mol	Joback Method
hf	34.66	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	51.37	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.841		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	524.06	K	Joback Method
tc	753.66	K	Joback Method
tf	332.04	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.53	J/mol×K	524.06	Joback Method
cpg	265.37	J/mol×K	562.33	Joback Method
cpg	276.44	J/mol×K	600.59	Joback Method
cpg	286.78	J/mol×K	638.86	Joback Method
cpg	296.41	J/mol×K	677.13	Joback Method
cpg	305.38	J/mol×K	715.39	Joback Method
cpg	313.73	J/mol×K	753.66	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=C13078790&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