Aniline, n-beta-chloroallyl-

Inchi: InChI=1S/C9H10ClN/c1-8(10)7-11-9-5-3-2-4-6-9/h2-6,11H,1,7H2
InchiKey: BIENNPBMRHEDOY-UHFFFAOYSA-N
Formula: C9H10ClN
SMILES: C=C(Cl)CNc1ccccc1
Mol. weight [g/mol]: 167.63
CAS: 15332-67-9

Physical Properties

Property code	Value	Unit	Source
gf	294.06	kJ/mol	Joback Method
hf	160.81	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	48.13	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.851		Crippen Method
mcvol	131.830	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
tb	516.16	K	Joback Method
tc	739.94	K	Joback Method
tf	284.47	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.33	J/mol×K	516.16	Joback Method
cpg	282.30	J/mol×K	553.46	Joback Method
cpg	294.37	J/mol×K	590.75	Joback Method
cpg	305.59	J/mol×K	628.05	Joback Method
cpg	315.99	J/mol×K	665.34	Joback Method
cpg	325.65	J/mol×K	702.64	Joback Method
cpg	334.59	J/mol×K	739.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15332679&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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