N-(2-Chloroethyl)benzamide

Other names: Benzamide, N-(2-chloroethyl)-
Inchi: InChI=1S/C9H10ClNO/c10-6-7-11-9(12)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,11,12)
InchiKey: FYQJUYCGPLFWQR-UHFFFAOYSA-N
Formula: C9H10ClNO
SMILES: O=C(NCCCl)c1ccccc1
Mol. weight [g/mol]: 183.63
CAS: 26385-07-9

Physical Properties

Property code	Value	Unit	Source
gf	85.85	kJ/mol	Joback Method
hf	-67.41	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	55.47	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.655		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	573.47	K	Joback Method
tc	796.67	K	Joback Method
tf	350.12	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.51	J/mol×K	573.47	Joback Method
cpg	315.62	J/mol×K	610.67	Joback Method
cpg	326.88	J/mol×K	647.87	Joback Method
cpg	337.34	J/mol×K	685.07	Joback Method
cpg	347.04	J/mol×K	722.27	Joback Method
cpg	356.01	J/mol×K	759.47	Joback Method
cpg	364.29	J/mol×K	796.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26385079&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