Cyclohexanecarboxamide, n-(2-chloroethyl)-

Inchi: InChI=1S/C9H16ClNO/c10-6-7-11-9(12)8-4-2-1-3-5-8/h8H,1-7H2,(H,11,12)
InchiKey: GMRFYVCWMWVBPT-UHFFFAOYSA-N
Formula: C9H16ClNO
SMILES: O=C(NCCCl)C1CCCCC1
Mol. weight [g/mol]: 189.68
CAS: 16813-44-8

Physical Properties

Property code	Value	Unit	Source
gf	-2.11	kJ/mol	Joback Method
hf	-249.62	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.922		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	566.34	K	Joback Method
tc	782.14	K	Joback Method
tf	331.08	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.36	J/mol×K	566.34	Joback Method
cpg	380.80	J/mol×K	602.31	Joback Method
cpg	396.23	J/mol×K	638.27	Joback Method
cpg	410.69	J/mol×K	674.24	Joback Method
cpg	424.21	J/mol×K	710.21	Joback Method
cpg	436.83	J/mol×K	746.18	Joback Method
cpg	448.57	J/mol×K	782.14	Joback Method

Sources

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=C16813448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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