2,2,2-Trichloro-n-cyclohexyl acetamide

Inchi: InChI=1S/C8H12Cl3NO/c9-8(10,11)7(13)12-6-4-2-1-3-5-6/h6H,1-5H2,(H,12,13)
InchiKey: JFRFGCASIOOBDA-UHFFFAOYSA-N
Formula: C8H12Cl3NO
SMILES: O=C(NC1CCCCC1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 244.55
CAS: 23144-68-5

Physical Properties

Property code	Value	Unit	Source
gf	-31.55	kJ/mol	Joback Method
hf	-269.21	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	58.87	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.805		Crippen Method
mcvol	160.990	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
tb	615.09	K	Joback Method
tc	856.87	K	Joback Method
tf	382.07	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.22	J/mol×K	615.09	Joback Method
cpg	388.55	J/mol×K	655.39	Joback Method
cpg	401.67	J/mol×K	695.68	Joback Method
cpg	413.64	J/mol×K	735.98	Joback Method
cpg	424.56	J/mol×K	776.28	Joback Method
cpg	434.48	J/mol×K	816.57	Joback Method
cpg	443.50	J/mol×K	856.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23144685&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