CCl3CH2N(CH3)2

Inchi: InChI=1S/C4H8Cl3N/c1-8(2)3-4(5,6)7/h3H2,1-2H3
InchiKey: UBTRQFXCMOCQLN-UHFFFAOYSA-N
Formula: C4H8Cl3N
SMILES: CN(C)CC(Cl)(Cl)Cl
Mol. weight [g/mol]: 176.47
CAS: 36726-94-0

Physical Properties

Property code	Value	Unit	Source
affp	912.80	kJ/mol	NIST Webbook
basg	882.00	kJ/mol	NIST Webbook
gf	60.63	kJ/mol	Joback Method
hf	-114.33	kJ/mol	Joback Method
hfus	14.31	kJ/mol	Joback Method
hvap	38.40	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.918		Crippen Method
mcvol	113.920	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	412.42	K	Joback Method
tc	613.56	K	Joback Method
tf	259.49	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.83	J/mol×K	412.42	Joback Method
cpg	202.43	J/mol×K	445.94	Joback Method
cpg	211.34	J/mol×K	479.47	Joback Method
cpg	219.59	J/mol×K	512.99	Joback Method
cpg	227.23	J/mol×K	546.51	Joback Method
cpg	234.29	J/mol×K	580.03	Joback Method
cpg	240.82	J/mol×K	613.56	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=C36726940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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