2,2,2-Trichloro-N,N-dimethylacetamide

Other names: Acetamide, 2,2,2-trichloro-N,N-dimethyl-
Trichloroacetamide, N,N-dimethyl-
Inchi: InChI=1S/C4H6Cl3NO/c1-8(2)3(9)4(5,6)7/h1-2H3
InchiKey: WGBMKQSRUSKSOM-UHFFFAOYSA-N
Formula: C4H6Cl3NO
SMILES: CN(C)C(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 190.46
CAS: 7291-33-0

Physical Properties

Property code	Value	Unit	Source
gf	-68.29	kJ/mol	Joback Method
hf	-226.91	kJ/mol	Joback Method
hfus	15.91	kJ/mol	Joback Method
hvap	45.15	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	1.445		Crippen Method
mcvol	115.490	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	504.50 ± 1.50	K	NIST Webbook
tc	679.39	K	Joback Method
tf	309.42	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.37	J/mol×K	466.29	Joback Method
cpg	213.78	J/mol×K	501.81	Joback Method
cpg	221.51	J/mol×K	537.32	Joback Method
cpg	228.58	J/mol×K	572.84	Joback Method
cpg	235.05	J/mol×K	608.35	Joback Method
cpg	240.96	J/mol×K	643.87	Joback Method
cpg	246.36	J/mol×K	679.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7291330&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