Acetamide, 2,2,2-trichloro-N-(4-methoxyphenyl)-

Other names: Acetamide, N-(4-methoxyphenyl)-2,2,2-trichloro-
Inchi: InChI=1S/C9H8Cl3NO2/c1-15-7-4-2-6(3-5-7)13-8(14)9(10,11)12/h2-5H,1H3,(H,13,14)
InchiKey: IFSVHMNTIRKVCD-UHFFFAOYSA-N
Formula: C9H8Cl3NO2
SMILES: COc1ccc(NC(=O)C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]: 268.52
CAS: 4257-81-2

Physical Properties

Property code	Value	Unit	Source
gf	-49.80	kJ/mol	Joback Method
hf	-251.33	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	66.02	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.004		Crippen Method
mcvol	168.050	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1866.00		NIST Webbook
tb	672.50	K	Joback Method
tc	913.89	K	Joback Method
tf	447.13	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.72	J/mol×K	672.50	Joback Method
cpg	383.78	J/mol×K	712.73	Joback Method
cpg	392.95	J/mol×K	752.96	Joback Method
cpg	401.26	J/mol×K	793.19	Joback Method
cpg	408.79	J/mol×K	833.43	Joback Method
cpg	415.59	J/mol×K	873.66	Joback Method
cpg	421.70	J/mol×K	913.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4257812&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume