Pentachlorophenyl dimethyl carbamate

Inchi: InChI=1S/C9H6Cl5NO2/c1-15(2)9(16)17-8-6(13)4(11)3(10)5(12)7(8)14/h1-2H3
InchiKey: YYZZEEYCOSFSTR-UHFFFAOYSA-N
Formula: C9H6Cl5NO2
SMILES: CN(C)C(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 337.41
CAS: 90418-41-0

Physical Properties

Property code	Value	Unit	Source
gf	-93.63	kJ/mol	Joback Method
hf	-305.88	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	74.34	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	5.014		Crippen Method
mcvol	192.530	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	732.78	K	Joback Method
tc	967.85	K	Joback Method
tf	534.44	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.93	J/mol×K	732.78	Joback Method
cpg	402.93	J/mol×K	771.96	Joback Method
cpg	410.28	J/mol×K	811.14	Joback Method
cpg	416.99	J/mol×K	850.31	Joback Method
cpg	423.07	J/mol×K	889.49	Joback Method
cpg	428.51	J/mol×K	928.67	Joback Method
cpg	433.33	J/mol×K	967.85	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=C90418410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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