2,4,5-Trichlorophenyl-n,n-dimethyl carbamate

Inchi: InChI=1S/C9H8Cl3NO2/c1-13(2)9(14)15-8-4-6(11)5(10)3-7(8)12/h3-4H,1-2H3
InchiKey: VCSDFCWFZZFAEC-UHFFFAOYSA-N
Formula: C9H8Cl3NO2
SMILES: CN(C)C(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 268.52
CAS: 6935-06-4

Physical Properties

Property code	Value	Unit	Source
gf	-50.51	kJ/mol	Joback Method
hf	-251.46	kJ/mol	Joback Method
hfus	30.34	kJ/mol	Joback Method
hvap	64.24	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.707		Crippen Method
mcvol	168.050	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
tb	647.96	K	Joback Method
tc	875.86	K	Joback Method
tf	449.56	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.77	J/mol×K	647.96	Joback Method
cpg	368.80	J/mol×K	685.94	Joback Method
cpg	378.14	J/mol×K	723.93	Joback Method
cpg	386.78	J/mol×K	761.91	Joback Method
cpg	394.76	J/mol×K	799.89	Joback Method
cpg	402.08	J/mol×K	837.88	Joback Method
cpg	408.77	J/mol×K	875.86	Joback Method

Sources

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=C6935064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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