2-Chloro-4-nitro-phenyl dimethyl carbamate

Inchi: InChI=1S/C9H9ClN2O4/c1-11(2)9(13)16-8-4-3-6(12(14)15)5-7(8)10/h3-5H,1-2H3
InchiKey: OELFGZWNLWXMBS-UHFFFAOYSA-N
Formula: C9H9ClN2O4
SMILES: CN(C)C(=O)Oc1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]: 244.63
CAS: 29285-59-4

Physical Properties

Property code	Value	Unit	Source
gf	18.53	kJ/mol	Joback Method
hf	-219.27	kJ/mol	Joback Method
hfus	33.70	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.309		Crippen Method
mcvol	160.990	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	719.96	K	Joback Method
tc	961.57	K	Joback Method
tf	520.81	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.91	J/mol×K	719.96	Joback Method
cpg	413.51	J/mol×K	760.23	Joback Method
cpg	423.21	J/mol×K	800.50	Joback Method
cpg	432.05	J/mol×K	840.76	Joback Method
cpg	440.06	J/mol×K	881.03	Joback Method
cpg	447.25	J/mol×K	921.30	Joback Method
cpg	453.67	J/mol×K	961.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29285594&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

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