tert-Butyl carbamate

Other names:	Carbamic acid, 1,1-dimethylethyl ester
	o-t-butyl carbamate
Inchi:	InChI=1S/C5H11NO2/c1-5(2,3)8-4(6)7/h1-3H3,(H2,6,7)
InchiKey:	LFKDJXLFVYVEFG-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	CC(C)(C)OC(N)=O
Mol. weight [g/mol]:	117.15
CAS:	4248-19-5

Physical Properties

Property code	Value	Unit	Source
gf	-173.41	kJ/mol	Joback Method
hf	-366.29	kJ/mol	Joback Method
hfus	9.28	kJ/mol	Joback Method
hvap	45.23	kJ/mol	Joback Method
log10ws	0.10		Aqueous Solubility Prediction Method
logp	0.880		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	459.39	K	Joback Method
tc	664.62	K	Joback Method
tf	303.95	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.64	J/mol×K	459.39	Joback Method
cpg	224.01	J/mol×K	493.60	Joback Method
cpg	233.84	J/mol×K	527.80	Joback Method
cpg	243.13	J/mol×K	562.01	Joback Method
cpg	251.91	J/mol×K	596.21	Joback Method
cpg	260.19	J/mol×K	630.42	Joback Method

cpg	267.99	J/mol×K	664.62	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4248195&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume