

Carbamic acid, t-butyl ester

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:	LFKDJXLFFVYVEFG-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	CC(C)(C)OC(N)=O
Mol. weight [g/mol]:	117.15

Physical Properties

Property code	Value	Unit	Source
hf	-556.76	kJ/mol	Cheméo Relay (1.0)
hfus	9.28	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Cheméo Relay (1.0)
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	411.30	K	Cheméo Relay (1.0)
tf	277.06	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4248195&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tf:	Normal melting (fusion) point

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