

Carbamic acid, N-methyl, t-butyl ester

Other names:	tert-Butyl methylcarbamate Carbamic acid, methyl, tert-butyl ester tert-Butyl N-methylcarbamate tert.-Butyl N-methyl carbamate
Inchi:	InChI=1S/C6H13NO2/c1-6(2,3)9-5(8)7-4/h1-4H3,(H,7,8)
InchiKey:	JHLVEBNWCCKSGY-UHFFFAOYSA-N
Formula:	C6H13NO2
SMILES:	CNC(=O)OC(C)(C)C
Mol. weight [g/mol]:	131.17
CAS:	16066-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-142.05	kJ/mol	Joback Method
hf	-367.25	kJ/mol	Joback Method
hfus	11.77	kJ/mol	Joback Method
hvap	43.25	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.141		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	935.00		NIST Webbook
rinpol	935.00		NIST Webbook
ripol	1392.00		NIST Webbook
tb	459.91	K	Joback Method
tc	652.80	K	Joback Method
tf	284.62	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.97	J/mol×K	459.91	Joback Method
cpg	255.67	J/mol×K	492.06	Joback Method

cpg	266.79	J/mol×K	524.21	Joback Method
cpg	277.36	J/mol×K	556.36	Joback Method
cpg	287.39	J/mol×K	588.51	Joback Method
cpg	296.89	J/mol×K	620.66	Joback Method
cpg	305.88	J/mol×K	652.80	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=C16066845&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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