

Carbamic acid, methyl, butyl ester

Other names:	Carbamic acid, N-methyl, butyl ester Butyl N-methyl carbamate
Inchi:	InChI=1S/C6H13NO2/c1-3-4-5-9-6(8)7-2/h3-5H2,1-2H3,(H,7,8)
InchiKey:	YAUWHXKOYHADTR-UHFFFAOYSA-N
Formula:	C6H13NO2
SMILES:	CCCCOC(O)=NC
Mol. weight [g/mol]:	131.17

Physical Properties

Property code	Value	Unit	Source
hf	-379.19	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	1.347		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1058.00		NIST Webbook
rinpol	1065.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	527.84	K	Joback Method
tc	709.29	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation 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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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