

Carbamic acid, methyl isobutyl ester

Other names:	Isobutyl N-methyl carbamate
Inchi:	InChI=1S/C6H13NO2/c1-5(2)4-9-6(8)7-3/h5H,4H2,1-3H3,(H,7,8)
InchiKey:	NKDJIJPGIVVJCN-UHFFFAOYSA-N
Formula:	C6H13NO2
SMILES:	CN=C(O)OCC(C)C
Mol. weight [g/mol]:	131.17

Physical Properties

Property code	Value	Unit	Source
hf	-384.47	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	1.203		Crippen Method
mvol	112.820	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
ripol	1525.00		NIST Webbook
tb	527.40	K	Joback Method
tc	712.52	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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