

Carbamic acid, N-(2-methylpropyl)-, 2-methylpropyl ester

Other names:	Isobutylcarbamate, N-isobutyl
Inchi:	InChI=1S/C9H19NO2/c1-7(2)5-10-9(11)12-6-8(3)4/h7-8H,5-6H2,1-4H3,(H,10,11)
InchiKey:	SHYVBTILSIXDJB-UHFFFAOYSA-N
Formula:	C9H19NO2
SMILES:	CC(C)CN=C(O)OCC(C)C
Mol. weight [g/mol]:	173.25
CAS:	178918-28-0

Physical Properties

Property code	Value	Unit	Source
hf	-451.67	kJ/mol	Joback Method
hvap	57.34	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	2.229		Crippen Method
mcvol	155.090	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
tb	595.60	K	Joback Method
tc	778.46	K	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=C178918280&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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