

Isobutyl nitrite

Other names:	(CH3)2CHCH2ONO Nitrous acid, 2-methylpropyl ester Nitrous acid, isobutyl ester IBN NCI-C61052
Inchi:	InChI=1S/C4H9NO2/c1-4(2)3-7-5-6/h4H,3H2,1-2H3
InchiKey:	APNSGVMLAYLYCT-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CC(C)CON=O
Mol. weight [g/mol]:	103.12
CAS:	542-56-3

Physical Properties

Property code	Value	Unit	Source
chl	-2675.00 ± 0.80	kJ/mol	NIST Webbook
hf	-151.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-186.00	kJ/mol	NIST Webbook
hvap	35.00	kJ/mol	NIST Webbook
log10ws	-1.53		Crippen Method
logp	1.340		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	576.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	544.00		NIST Webbook
ripol	725.00		NIST Webbook
ripol	725.00		NIST Webbook
tb	340.30 ± 0.50	K	NIST Webbook
tb	340.65 ± 2.00	K	NIST Webbook
tb	340.20	K	NIST Webbook
tb	340.00 ± 1.00	K	NIST Webbook
tc	548.96	K	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542563&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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