n-Butyl nitrite

Other names:	Nitrous acid, butyl ester
	Butyl nitrite
	n-C4H9ONO
	Nitrous acid, n-butyl ester
	NBN
	NCI-C56553
	UN 2351
	Butyl ester of nitrous acid
	NSC 8426
Inchi:	InChI=1S/C4H9NO2/c1-2-3-4-7-5-6/h2-4H2,1H3
InchiKey:	JQJPBYFTQAANLE-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CCCCON=O
Mol. weight [g/mol]:	103.12
CAS:	544-16-1

Physical Properties

Property code	Value	Unit	Source
chl	-2678.00 ± 0.80	kJ/mol	NIST Webbook
hf	-146.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-182.00	kJ/mol	NIST Webbook
hvap	37.00	kJ/mol	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.485		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	608.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	590.00		NIST Webbook
tb	351.00 ± 1.00	K	NIST Webbook
tb	351.20	K	NIST Webbook
tc	545.44	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=C544161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature