t-Butyl nitrite

Other names:	(CH3)3CONO
	tert-Butyl nitrite
	Nitrous acid, 1,1-dimethylethyl ester
	Nitrous acid, t-butyl ester
	«alpha»,«alpha»-Dimethylethyl nitrite
	tert.-Butyl nitrite
Inchi:	InChI=1S/C4H9NO2/c1-4(2,3)7-5-6/h1-3H3
InchiKey:	IOGXOCVLYRDXLW-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CC(C)(C)ON=O
Mol. weight [g/mol]:	103.12
CAS:	540-80-7

Physical Properties

Property code	Value	Unit	Source
affp	863.90	kJ/mol	NIST Webbook
basg	831.40	kJ/mol	NIST Webbook
chl	-2654.00 ± 3.00	kJ/mol	NIST Webbook
hf	-172.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-206.00	kJ/mol	NIST Webbook
hvap	34.00	kJ/mol	NIST Webbook
log10ws	-1.88		Crippen Method
logp	1.483		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	533.00		NIST Webbook
ripol	720.00		NIST Webbook
tb	335.00 ± 1.00	K	NIST Webbook
tb	336.00	K	NIST Webbook
tb	336.20	K	NIST Webbook
tc	553.55	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	30.80	kJ/mol	302.00	NIST Webbook

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=C540807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hvapt:	Enthalpy of vaporization at a given temperature
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