tert-Butyl Hydroperoxide

Other names:	Hydroperoxide, 1,1-dimethylethyl
	Cadox TBH
	Perbutyl H
	2-Hydroperoxy-2-methylpropane
	1,1-Dimethylethyl hydroperoxide
	tert-C4H9OOH
	tert-Butyl hydrogen peroxide
	Hydroperoxide, tert-butyl
	Hydroperoxyde de butyle tertiaire
	Slimicide DE-488
	Terc. butylhydroperoxid
	Trigonox A-75
	TBHP-70
	Trigonox A-W70
	t-Butylhydroperoxide
	Aztec t-butyl Hydroperoxide-70, Aq
	Dimethylethyl hydroperoxide
	T-Hydro
	TBHP
	Tertiary-butyl hydroperoxide
	NSC 672
Inchi:	InChI=1S/C4H10O2/c1-4(2,3)6-5/h5H,1-3H3
InchiKey:	CIHOLLKRGTVIJN-UHFFFAOYSA-N
Formula:	C4H10O2
SMILES:	CC(C)(C)OO
Mol. weight [g/mol]:	90.12
CAS:	75-91-2

Physical Properties

Property code	Value	Unit	Source
chl	-2736.00 ± 1.00	kJ/mol	NIST Webbook
chl	-2710.00 ± 5.00	kJ/mol	NIST Webbook
chl	-2737.00	kJ/mol	NIST Webbook
gf	-256.18	kJ/mol	Joback Method
hf	-246.00 ± 5.00	kJ/mol	NIST Webbook
hf	-234.90	kJ/mol	NIST Webbook

hfl	-294.00 ± 5.00	kJ/mol	NIST Webbook
hfus	3.98	kJ/mol	Joback Method
hvap	47.70 ± 0.20	kJ/mol	NIST Webbook
hvap	48.10	kJ/mol	NIST Webbook
hvap	48.00	kJ/mol	NIST Webbook
ie	10.24	eV	NIST Webbook
log10ws	-1.01		Crippen Method
logp	1.274		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	402.29	K	Joback Method
tc	575.17	K	Joback Method
tf	220.31	K	Joback Method
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.68	J/mol×K	575.17	Joback Method
cpg	193.32	J/mol×K	546.35	Joback Method
cpg	186.67	J/mol×K	517.54	Joback Method
cpg	179.70	J/mol×K	488.73	Joback Method
cpg	172.42	J/mol×K	459.92	Joback Method
cpg	164.80	J/mol×K	431.10	Joback Method
cpg	156.85	J/mol×K	402.29	Joback Method
dvisc	0.0885825	Pa×s	220.31	Joback Method
dvisc	0.0003005	Pa×s	402.29	Joback Method
dvisc	0.0005268	Pa×s	371.96	Joback Method
dvisc	0.0010203	Pa×s	341.63	Joback Method
dvisc	0.0022475	Pa×s	311.30	Joback Method
dvisc	0.0058716	Pa×s	280.97	Joback Method
dvisc	0.0193527	Pa×s	250.64	Joback Method
hvapt	46.57	kJ/mol	153.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C75912&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume