Di-tert-butyl peroxide

Other names:	(tert-C4H9O)2
	Bis(1,1-dimethylethyl) peroxide
	Bis(tert-butyl) peroxide
	Cadox
	Cadox TBP
	DTBP
	Di-t-butyl peroxide
	Di-tert-butyl peroxyde
	Di-tert-butylperoxid
	Di-tertiary-butyl peroxide
	Interox DTB
	Kayabutyl D
	NSC 673
	Perbutyl D
	Perossido di butile terziario
	Peroxide, bis(1,1-dimethylethyl)
	Peroxide, bis-tert-butyl-
	Peroxide, tert-butyl-
	Peroxyde de butyle tertiaire
	Trigonox B
	t-Butyl peroxide
	t-butyl peroxide bis(1,1-di-methylethyl)peroxide
	tert-Butyl peroxide
Inchi:	InChI=1S/C8H18O2/c1-7(2,3)9-10-8(4,5)6/h1-6H3
InchiKey:	LSXWFXONGKSEMY-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CC(C)(C)OOC(C)(C)C
Mol. weight [g/mol]:	146.23
CAS:	110-05-4

Physical Properties

Property code	Value	Unit	Source
chl	-5339.80 ± 1.60	kJ/mol	NIST Webbook
chl	-5336.30	kJ/mol	NIST Webbook
chl	-5339.60 ± 0.80	kJ/mol	NIST Webbook
chl	-5334.60	kJ/mol	NIST Webbook

chl	-5326.00	kJ/mol	NIST Webbook
gf	-187.84	kJ/mol	Joback Method
hf	-341.00	kJ/mol	NIST Webbook
hf	-343.00	kJ/mol	NIST Webbook
hf	-340.80	kJ/mol	NIST Webbook
hfl	-380.80 ± 2.00	kJ/mol	NIST Webbook
hfl	-381.00	kJ/mol	NIST Webbook
hfl	-385.00	kJ/mol	NIST Webbook
hfus	4.02	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
ie	8.78	eV	NIST Webbook
ie	8.78	eV	NIST Webbook
log10ws	-2.56		Crippen Method
logp	2.532		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
tb	382.70	K	NIST Webbook
tc	606.65	K	Joback Method
tf	229.22	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.80	J/mol×K	513.74	Joback Method
cpg	367.29	J/mol×K	606.65	Joback Method
cpg	355.43	J/mol×K	575.68	Joback Method
cpg	342.94	J/mol×K	544.71	Joback Method
cpg	286.25	J/mol×K	420.82	Joback Method
cpg	301.47	J/mol×K	451.79	Joback Method
cpg	315.98	J/mol×K	482.76	Joback Method
dvisc	0.0002166	Pa×s	420.82	Joback Method
dvisc	0.0007582	Pa×s	325.02	Joback Method
dvisc	0.0004634	Pa×s	356.95	Joback Method
dvisc	0.0003070	Pa×s	388.89	Joback Method
dvisc	0.0075653	Pa×s	229.22	Joback Method
dvisc	0.0029132	Pa×s	261.15	Joback Method
dvisc	0.0013811	Pa×s	293.09	Joback Method
hvapt	31.05	kJ/mol	253.00	NIST Webbook
hvapt	31.00	kJ/mol	328.50	NIST Webbook
hvapt	32.00	kJ/mol	278.50	NIST Webbook

hvapt	37.00	kJ/mol	333.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	9.64980e+00
Coeff. B	-2.14376e+03
Coeff. C	-5.29490e+01
Temperature range (K), min.	281.93
Temperature range (K), max.	547.09

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C110054&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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume