Peroxide, 1,1-dimethylethyl 1-methyl-1-phenylethyl

Other names: tert-Butyl «alpha»,«alpha»-dimethylbenzyl peroxide
Peroxide, tert-butyl «alpha»,«alpha»-dimethylbenzyl
tert-Butyl cumene peroxide
tert-Butyl cumyl peroxide
Cumyl tert-butyl peroxide
Kayabutyl C
Trigonox T
1,1-Dimethylethyl 1-methyl-1-phenylethyl peroxide
Luperco 801-XL
t-Butyl cumyl peroxide
Luperox 801

Inchi: InChI=1S/C13H20O2/c1-12(2,3)14-15-13(4,5)11-9-7-6-8-10-11/h6-10H,1-5H3

InchiKey: BIISIZOQPWZPPS-UHFFFAOYSA-N

Formula: C13H20O2

SMILES: CC(C)(C)OOC(C)(C)c1ccccc1

Mol. weight [g/mol]: 208.30

CAS: 3457-61-2

Physical Properties

Property code	Value	Unit	Source
chl	-7710.50 ± 5.80	kJ/mol	NIST Webbook
gf	-33.33	kJ/mol	Joback Method
hf	-357.06	kJ/mol	Joback Method
hfl	-263.00 ± 5.80	kJ/mol	NIST Webbook
hfus	11.02	kJ/mol	Joback Method
hvap	49.04	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.668		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
tb	561.90	K	Joback Method
tc	779.45	K	Joback Method
tf	311.99	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.17	J/mol×K	779.45	Joback Method
cpg	535.92	J/mol×K	743.19	Joback Method
cpg	521.67	J/mol×K	706.93	Joback Method
cpg	506.34	J/mol×K	670.68	Joback Method
cpg	489.90	J/mol×K	634.42	Joback Method
cpg	472.27	J/mol×K	598.16	Joback Method
cpg	453.41	J/mol×K	561.90	Joback Method
dvisc	0.0028405	Pa×s	311.99	Joback Method
dvisc	0.0001081	Pa×s	561.90	Joback Method
dvisc	0.0001498	Pa×s	520.25	Joback Method
dvisc	0.0002199	Pa×s	478.60	Joback Method
dvisc	0.0003471	Pa×s	436.94	Joback Method
dvisc	0.0006035	Pa×s	395.29	Joback Method
dvisc	0.0011951	Pa×s	353.64	Joback Method
hvapt	69.10 ± 1.40	kJ/mol	294.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3457612&Units=SI
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

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
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