

Tert-butyl cumyl peroxide

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

Physical Properties

Property code	Value	Unit	Source
af	0.4898		Cheméo Relay (1.0)
chl	-7710.50 ± 5.80	kJ/mol	NIST Webbook
hf	-174.24	kJ/mol	Cheméo Relay (1.0)
hfl	-263.00 ± 5.80	kJ/mol	NIST Webbook
hfus	11.01	kJ/mol	Joback Method
hvap	64.16	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-3.22		Cheméo Relay (1.0)
logp	3.668		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
tb	496.41	K	Cheméo Relay (1.0)
tc	703.17	K	Cheméo Relay (1.0)
tf	301.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3457612&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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