1,1-Dimethyl-1-methyl-1-[(4-methylethyl)phenyl]et peroxide

Other names: Peroxide, 1,1-dimethylethyl 1-methyl-1-[4-(1-methylethyl)phenyl]ethyl
Inchi: InChI=1S/C16H26O2/c1-12(2)13-8-10-14(11-9-13)16(6,7)18-17-15(3,4)5/h8-12H,1-7H3
InchiKey: QGABUHGYHVKOCM-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CC(C)c1ccc(C(C)(C)OOC(C)(C)C)cc1
Mol. weight [g/mol]: 250.38
CAS: 52031-72-8

Physical Properties

Property code	Value	Unit	Source
chl	-9659.90 ± 5.00	kJ/mol	NIST Webbook
gf	-20.14	kJ/mol	Joback Method
hf	-435.73	kJ/mol	Joback Method
hfl	-352.10 ± 5.00	kJ/mol	NIST Webbook
hfus	14.87	kJ/mol	Joback Method
hvap	55.99	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.792		Crippen Method
mcvol	224.280	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
tb	635.08	K	Joback Method
tc	847.08	K	Joback Method
tf	343.32	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.29	J/mol×K	847.08	Joback Method
cpg	609.65	J/mol×K	635.08	Joback Method
cpg	629.73	J/mol×K	670.41	Joback Method
cpg	648.54	J/mol×K	705.75	Joback Method
cpg	666.15	J/mol×K	741.08	Joback Method
cpg	682.60	J/mol×K	776.42	Joback Method

cpg	697.97	J/mol×K	811.75	Joback Method
dvisc	0.0000656	Pa×s	635.08	Joback Method
dvisc	0.0020216	Pa×s	343.32	Joback Method
dvisc	0.0008009	Pa×s	391.95	Joback Method
dvisc	0.0003892	Pa×s	440.57	Joback Method
dvisc	0.0002184	Pa×s	489.20	Joback Method
dvisc	0.0001360	Pa×s	537.83	Joback Method
dvisc	0.0000916	Pa×s	586.45	Joback Method
hvapt	73.30 ± 5.00	kJ/mol	307.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52031728&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

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