Hydroperoxide, 1-methyl-1-phenylethyl

Other names:	1-Methyl-1-phenylethyl hydroperoxide
	7-Cumyl hydroperoxide
	7-Hydroperoxykumen
	CHP
	CHP-158
	CHP-5
	Cumeenhydroperoxyde
	Cumene hydroperoxide
	Cument hydroperoxide
	Cumenyl hydroperoxide
	Cumolhydroperoxid
	Cumyl hydroperoxide
	Hydroperoxide, «alpha»,«alpha»-dimethylbenzyl
	Hydroperoxide, Â«alphaÂ»,Â«alphaÂ»-dimethylbenzyl
	Hydroperoxyde de cumene
	Hydroperoxyde de cumyle
	Hyperiz
	Idroperossido di cumene
	Idroperossido di cumolo
	Isopropylbenzene hydroperoxide
	Kumenylhydroperoxid
	Percumyl H
	Rcra waste number U096
	Trigonox K 80
	Trigonox K-95
	Trigonox R 239A
	UN 2116
	«alpha»,«alpha»-Dimethylbenzyl hydroperoxide
	«alpha»-Cumene hydroperoxide
	«alpha»-Cumyl hydroperoxide
	Â«alphaÂ»,Â«alphaÂ»-Dimethylbenzyl hydroperoxide
	Â«alphaÂ»-Cumene hydroperoxide
	Â«alphaÂ»-Cumyl hydroperoxide
Inchi:	InChI=1S/C9H12O2/c1-9(2,11-10)8-6-4-3-5-7-8/h3-7,10H,1-2H3
InchiKey:	YQHLDYVWEZKEOX-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CC(C)(OO)c1ccccc1
Mol. weight [g/mol]:	152.19
CAS:	80-15-9

Physical Properties

Property code	Value	Unit	Source
chl	-5108.20 ± 6.70	kJ/mol	NIST Webbook
gf	-101.67	kJ/mol	Joback Method
hf	-78.70 ± 6.70	kJ/mol	NIST Webbook
hfl	-149.00 ± 6.70	kJ/mol	NIST Webbook
hfs	-192.00	kJ/mol	NIST Webbook
hfus	10.97	kJ/mol	Joback Method
hvap	69.90	kJ/mol	NIST Webbook
hvap	69.90 ± 0.20	kJ/mol	NIST Webbook
hvap	70.30	kJ/mol	NIST Webbook
log10ws	-2.26		Crippen Method
logp	2.411		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	543.37	K	Joback Method
tc	748.48	K	Joback Method
tf	303.08	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.53	J/mol×K	543.37	Joback Method
cpg	305.74	J/mol×K	577.56	Joback Method
cpg	317.17	J/mol×K	611.74	Joback Method
cpg	327.86	J/mol×K	645.93	Joback Method
cpg	337.84	J/mol×K	680.11	Joback Method
cpg	347.17	J/mol×K	714.30	Joback Method
cpg	355.85	J/mol×K	748.48	Joback Method
dvisc	0.0105883	Pa×s	303.08	Joback Method
dvisc	0.0030015	Pa×s	343.13	Joback Method
dvisc	0.0011074	Pa×s	383.18	Joback Method
dvisc	0.0004934	Pa×s	423.23	Joback Method
dvisc	0.0002528	Pa×s	463.27	Joback Method
dvisc	0.0001441	Pa×s	503.32	Joback Method
dvisc	0.0000892	Pa×s	543.37	Joback Method
hvapt	74.00	kJ/mol	368.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.70	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.07891e+01
Coeff. B	-1.96802e+03
Coeff. C	-1.68886e+02
Temperature range (K), min.	356.29
Temperature range (K), max.	528.17

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80159&Units=SI

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

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
hfs:	Solid 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume