

8-hydroperoxy-p-cymene

Inchi:	InChI=1S/C10H14O2/c1-8-4-6-9(7-5-8)10(2,3)12-11/h4-7,11H,1-3H3
InchiKey:	YCCHNFGPIFYNTF-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	Cc1ccc(C(C)(C)OO)cc1
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
gf	-102.88	kJ/mol	Joback Method
hf	-317.87	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hvap	58.59	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.720		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinsol	1321.00		NIST Webbook
tb	571.23	K	Joback Method
tc	774.30	K	Joback Method
tf	326.87	K	Joback Method
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.92	J/molxK	571.23	Joback Method
cpg	351.63	J/molxK	605.08	Joback Method
cpg	363.58	J/molxK	638.92	Joback Method
cpg	374.81	J/molxK	672.77	Joback Method
cpg	385.34	J/molxK	706.61	Joback Method
cpg	395.21	J/molxK	740.46	Joback Method
cpg	404.46	J/molxK	774.30	Joback Method
dvisc	0.0054090	Paxs	326.87	Joback Method
dvisc	0.0017576	Paxs	367.60	Joback Method

dvisc	0.0007147	Paxs	408.32	Joback Method
dvisc	0.0003421	Paxs	449.05	Joback Method
dvisc	0.0001851	Paxs	489.78	Joback Method
dvisc	0.0001101	Paxs	530.50	Joback Method
dvisc	0.0000705	Paxs	571.23	Joback Method

Sources

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=R342771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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