

p-mentha-1,8-dien-4-yl-hydroperoxide

Inchi:	InChI=1S/C10H16O2/c1-8(2)10(12-11)6-4-9(3)5-7-10/h11H,1,3-7H2,2H3
InchiKey:	ZZBKPOOBGMOEIO-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	<chem>C=C1CCC(OO)(C(=C)C)CC1</chem>
Mol. weight [g/mol]:	168.23

Physical Properties

Property code	Value	Unit	Source
gf	-57.17	kJ/mol	Joback Method
hf	-264.74	kJ/mol	Joback Method
hfus	8.72	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.921		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinsol	1327.00		NIST Webbook
tb	558.31	K	Joback Method
tc	758.83	K	Joback Method
tf	314.75	K	Joback Method
vc	0.529	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.53	J/mol×K	558.31	Joback Method
cpg	368.73	J/mol×K	591.73	Joback Method
cpg	382.15	J/mol×K	625.15	Joback Method
cpg	394.88	J/mol×K	658.57	Joback Method
cpg	407.00	J/mol×K	691.99	Joback Method
cpg	418.59	J/mol×K	725.41	Joback Method
cpg	429.73	J/mol×K	758.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R339181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

cpg:	Ideal gas heat capacity
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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