

(E)-p-mentha-1(7),8-dien-2-hydroperoxide

Inchi:

InChI=1S/C10H16O2/c1-7(2)9-5-4-8(3)10(6-9)12-11/h9-11H,1,3-6H2,2H3/t9-,10+/m1/s1

InchiKey:

CSOZFPOODGAASP-ZJUUVORDSA-N

Formula:

C10H16O2

SMILES:

C=C(C)C1CCC(=C)C(OO)C1

Mol. weight [g/mol]:

168.23

Physical Properties

Property code	Value	Unit	Source
gf	-59.39	kJ/mol	Joback Method
hf	-300.32	kJ/mol	Joback Method
hfus	16.09	kJ/mol	Joback Method
hvap	56.63	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.777		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1338.00		NIST Webbook
rinpol	1338.00		NIST Webbook
tb	553.40	K	Joback Method
tc	746.37	K	Joback Method
tf	286.61	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.90	J/mol×K	553.40	Joback Method
cpg	371.78	J/mol×K	585.56	Joback Method
cpg	385.96	J/mol×K	617.72	Joback Method
cpg	399.45	J/mol×K	649.88	Joback Method
cpg	412.26	J/mol×K	682.05	Joback Method
cpg	424.38	J/mol×K	714.21	Joback Method
cpg	435.84	J/mol×K	746.37	Joback Method

Sources

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=R339161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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