

(2S,4R)-p-Mentha-6,8-diene 2-hydroperoxide

Other names:	(E)-p-mentha-6,8-dien-2-hydroperoxide
Inchi:	InChI=1S/C10H16O2/c1-7(2)9-5-4-8(3)10(6-9)12-11/h4,9-11H,1,5-6H2,2-3H3
InchiKey:	VAVIEVIKILAXDG-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	<chem>C=C(C)C1CC=C(C)C(OO)C1</chem>
Mol. weight [g/mol]:	168.23

Physical Properties

Property code	Value	Unit	Source
gf	-92.14	kJ/mol	Joback Method
hf	-338.25	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.777		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1381.00		NIST Webbook
tb	558.38	K	Joback Method
tc	752.53	K	Joback Method
tf	286.21	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.69	J/molxK	558.38	Joback Method
cpg	372.41	J/molxK	590.74	Joback Method
cpg	386.44	J/molxK	623.10	Joback Method
cpg	399.77	J/molxK	655.45	Joback Method
cpg	412.41	J/molxK	687.81	Joback Method
cpg	424.38	J/molxK	720.17	Joback Method
cpg	435.69	J/molxK	752.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292743&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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