

cis-2-t-butyl-peroxy-p-mentha-1(7),8-diene

Inchi:	InChI=1S/C14H24O2/c1-10(2)12-8-7-11(3)13(9-12)15-16-14(4,5)6/h12-13H,1,3,7-9H2,2,
InchiKey:	RGCDJHCIWRIPJR-STQMWFEESA-N
Formula:	C14H24O2
SMILES:	C=C(C)C1CCC(=C)C(OOC(C)(C)C)C1
Mol. weight [g/mol]:	224.34

Physical Properties

Property code	Value	Unit	Source
gf	8.95	kJ/mol	Joback Method
hf	-371.62	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	49.97	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.034		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinsol	1300.00		NIST Webbook
tb	571.93	K	Joback Method
tc	776.20	K	Joback Method
tf	295.52	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.53	J/molxK	571.93	Joback Method
cpg	541.75	J/molxK	605.98	Joback Method
cpg	561.84	J/molxK	640.02	Joback Method
cpg	580.84	J/molxK	674.07	Joback Method
cpg	598.75	J/molxK	708.11	Joback Method
cpg	615.61	J/molxK	742.16	Joback Method
cpg	631.43	J/molxK	776.20	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=R402269&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
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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