

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H24O2/c1-10(2)12-8-7-11(3)13(9-12)15-16-14(4,5)6/h7-8,11-13H,1,9H2,2-

NGRCCIIMLAFQTKF-SPOOISQMSA-N

C14H24O2

C=C(C)C1C=CC(C)C(OOC(C)(C)C)C1

224.34

Physical Properties

Property code	Value	Unit	Source
gf	-21.88	kJ/mol	Joback Method
hf	-418.42	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	49.80	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.890		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
tb	567.26	K	Joback Method
tc	771.59	K	Joback Method
tf	278.36	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.94	J/mol×K	567.26	Joback Method
cpg	543.73	J/mol×K	601.32	Joback Method
cpg	564.35	J/mol×K	635.37	Joback Method
cpg	583.84	J/mol×K	669.43	Joback Method
cpg	602.20	J/mol×K	703.48	Joback Method
cpg	619.48	J/mol×K	737.54	Joback Method
cpg	635.69	J/mol×K	771.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R402254&Units=SI

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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