

6-t-butyl-peroxy-p-mentha-1,8-diene

Inchi:	InChI=1S/C14H24O2/c1-10(2)12-8-7-11(3)13(9-12)15-16-14(4,5)6/h7,12-13H,1,8-9H2,2-
InchiKey:	TUOFQQLUAFJSET-UHFFFAOYSA-N
Formula:	C14H24O2
SMILES:	C=C(C)C1CC=C(C)C(OOC(C)(C)C)C1
Mol. weight [g/mol]:	224.34

Physical Properties

Property code	Value	Unit	Source
gf	-23.80	kJ/mol	Joback Method
hf	-409.55	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.034		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	1327.00		NIST Webbook
rinpol	1327.00		NIST Webbook
tb	576.91	K	Joback Method
tc	782.36	K	Joback Method
tf	295.12	K	Joback Method
vc	0.745	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.07	J/mol×K	576.91	Joback Method
cpg	543.10	J/mol×K	611.15	Joback Method
cpg	563.00	J/mol×K	645.39	Joback Method
cpg	581.80	J/mol×K	679.64	Joback Method
cpg	599.53	J/mol×K	713.88	Joback Method
cpg	616.20	J/mol×K	748.12	Joback Method
cpg	631.84	J/mol×K	782.36	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=R402249&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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