(+)-(1R,4R,6R,7R,10S)-Muurolan-4,7-peroxide

Inchi: InChI=1S/C15H26O2/c1-9(2)15-8-7-10(3)12-6-5-11(4)14(13(12)15)16-17-15/h9-14H,5-8H
InchiKey: HPLUFHNNBOHIAJ-PNJKBWKFSA-N
Formula: C15H26O2
SMILES: CC1CCC2(C(C)C)OOC3C(C)CCC1C32
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	18.07	kJ/mol	Joback Method
hf	-468.07	kJ/mol	Joback Method
hfus	32.06	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.804		Crippen Method
mcvol	201.370	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		NIST Webbook
tb	615.32	K	Joback Method
tc	836.44	K	Joback Method
tf	351.39	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.90	J/mol×K	615.32	Joback Method
cpg	625.04	J/mol×K	652.17	Joback Method
cpg	647.72	J/mol×K	689.03	Joback Method
cpg	669.11	J/mol×K	725.88	Joback Method
cpg	689.38	J/mol×K	762.74	Joback Method
cpg	708.70	J/mol×K	799.59	Joback Method
cpg	727.25	J/mol×K	836.44	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=R561294&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume