(+)-Muurolan-4,7-peroxide

Inchi: InChI=1S/C15H26O2/c1-10(2)15-8-5-11(3)12-6-7-14(4,16-17-15)9-13(12)15/h10-13H,5-9
InchiKey: IGPMTDORMOJTHZ-FKQQDJLNSA-N
Formula: C15H26O2
SMILES: CC1CCC2(C(C)C)OOC3(C)CCC1C2C3
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	20.29	kJ/mol	Joback Method
hf	-432.49	kJ/mol	Joback Method
hfus	24.69	kJ/mol	Joback Method
hvap	54.95	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.948		Crippen Method
mcvol	201.370	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1485.00		NIST Webbook
tb	620.23	K	Joback Method
tc	849.95	K	Joback Method
tf	379.53	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.39	J/mol×K	620.23	Joback Method
cpg	620.95	J/mol×K	658.52	Joback Method
cpg	643.13	J/mol×K	696.80	Joback Method
cpg	664.23	J/mol×K	735.09	Joback Method
cpg	684.56	J/mol×K	773.38	Joback Method
cpg	704.41	J/mol×K	811.67	Joback Method
cpg	724.09	J/mol×K	849.95	Joback Method

Sources

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=R411337&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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