

7,10-Epoxy-10-hydroxysalvianane

Inchi:	InChI=1S/C15H26O2/c1-10(2)11-5-6-14(4)12(11)9-13(3)7-8-15(14,16)17-13/h10-12,16H
InchiKey:	WJRIMKOXIVMKTM-WQNPGBKJSA-N
Formula:	C15H26O2
SMILES:	CC(C)C1CCC2(C)C1CC1(C)CCC2(O)O1
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-23.80	kJ/mol	Joback Method
hf	-431.32	kJ/mol	Joback Method
hfus	16.60	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.336		Crippen Method
mcvol	201.370	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1643.00		NIST Webbook
tb	681.43	K	Joback Method
tc	896.88	K	Joback Method
tf	441.20	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.32	J/molxK	681.43	Joback Method
cpg	647.61	J/molxK	717.34	Joback Method
cpg	666.42	J/molxK	753.25	Joback Method
cpg	685.08	J/molxK	789.15	Joback Method
cpg	703.94	J/molxK	825.06	Joback Method
cpg	723.34	J/molxK	860.97	Joback Method
cpg	743.64	J/molxK	896.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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