2,2,6,9-Tetramethyl-3,4,6a,7-tetrahydro-2H-3,9a-m

Other names: Guaia-3,9-diene 5,11-oxide
Inchi: InChI=1S/C15H22O/c1-10-5-7-12-9-15(16-14(12,3)4)11(2)6-8-13(10)15/h5-6,12-13H,7-9
InchiKey: KVJMJCYPKZHEPD-RMTCENKZSA-N
Formula: C15H22O
SMILES: CC1=CCC2CC3(OC2(C)C)C(C)=CCC13
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	157.22	kJ/mol	Joback Method
hf	-182.25	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.857		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1518.00		NIST Webbook
tb	606.67	K	Joback Method
tc	840.69	K	Joback Method
tf	398.76	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.90	J/mol×K	606.67	Joback Method
cpg	539.75	J/mol×K	645.67	Joback Method
cpg	559.32	J/mol×K	684.68	Joback Method
cpg	577.94	J/mol×K	723.68	Joback Method
cpg	595.91	J/mol×K	762.68	Joback Method
cpg	613.56	J/mol×K	801.69	Joback Method
cpg	631.20	J/mol×K	840.69	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=R407759&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

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