ent-7-Hydroxy-eudesm-4-en-6-one

Inchi: InChI=1S/C15H24O2/c1-10(2)15(17)9-8-14(4)7-5-6-11(3)12(14)13(15)16/h10,17H,5-9H2
InchiKey: ZANHXCFRKGGJIZ-MLCCFXAWSA-N
Formula: C15H24O2
SMILES: CC1=C2C(=O)C(O)(C(C)C)CCC2(C)CCC1
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-113.61	kJ/mol	Joback Method
hf	-461.86	kJ/mol	Joback Method
hfus	10.40	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.243		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1672.00		NIST Webbook
tb	742.32	K	Joback Method
tc	966.16	K	Joback Method
tf	468.25	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.48	J/mol×K	742.32	Joback Method
cpg	644.35	J/mol×K	779.63	Joback Method
cpg	662.84	J/mol×K	816.93	Joback Method
cpg	681.18	J/mol×K	854.24	Joback Method
cpg	699.58	J/mol×K	891.55	Joback Method
cpg	718.25	J/mol×K	928.86	Joback Method
cpg	737.41	J/mol×K	966.16	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=R413368&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