6-«beta»-Hydroxy-4(15)-eudesmen-1-one

Inchi: InChI=1S/C15H24O2/c1-9(2)11-7-8-15(4)12(16)6-5-10(3)13(15)14(11)17/h9,11,13-14,17
InchiKey: GCPDRNZIBLNTCH-UQOMUDLDSA-N
Formula: C15H24O2
SMILES: C=C1CCC(=O)C2(C)CCC(C(C)C)C(O)C12
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-81.16	kJ/mol	Joback Method
hf	-468.38	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.955		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
ripol	2660.00		NIST Webbook
tb	722.78	K	Joback Method
tc	937.91	K	Joback Method
tf	423.75	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.52	J/mol×K	722.78	Joback Method
cpg	654.98	J/mol×K	758.64	Joback Method
cpg	673.51	J/mol×K	794.49	Joback Method
cpg	691.22	J/mol×K	830.35	Joback Method
cpg	708.20	J/mol×K	866.20	Joback Method
cpg	724.57	J/mol×K	902.06	Joback Method
cpg	740.40	J/mol×K	937.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R561249&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume