4-«beta»-H-Eudesmen-11(13)-ene-4,12-diol

Inchi: InChI=1S/C15H26O2/c1-11(10-16)12-5-8-14(2)6-4-7-15(3,17)13(14)9-12/h12-13,16-17H
InchiKey: RMARCXQAHOJNRB-AVOUXACISA-N
Formula: C15H26O2
SMILES: C=C(CO)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-72.23	kJ/mol	Joback Method
hf	-430.99	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	79.35	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.892		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1909.00		NIST Webbook
tb	745.22	K	Joback Method
tc	946.40	K	Joback Method
tf	425.85	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.50	J/mol×K	745.22	Joback Method
cpg	680.15	J/mol×K	778.75	Joback Method
cpg	697.45	J/mol×K	812.28	Joback Method
cpg	714.57	J/mol×K	845.81	Joback Method
cpg	731.70	J/mol×K	879.34	Joback Method
cpg	749.02	J/mol×K	912.87	Joback Method
cpg	766.74	J/mol×K	946.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R572868&Units=SI
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

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