Eudesm-6-en-1«beta»,4«beta»-diol (Isoplodiol)

Inchi: InChI=1S/C15H26O2/c1-10(2)11-5-7-14(3)12(9-11)15(4,17)8-6-13(14)16/h9-10,12-13,16
InchiKey: RGIVMNUHSHEEPN-WIGRTHMWSA-N
Formula: C15H26O2
SMILES: CC(C)C1=CC2C(C)(O)CCC(O)C2(C)CC1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-133.63	kJ/mol	Joback Method
hf	-505.60	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.891		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
ripol	2550.00		NIST Webbook
ripol	2550.00		NIST Webbook
tb	752.36	K	Joback Method
tc	953.34	K	Joback Method
tf	439.85	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.47	J/mol×K	752.36	Joback Method
cpg	679.86	J/mol×K	785.86	Joback Method
cpg	696.94	J/mol×K	819.35	Joback Method
cpg	713.89	J/mol×K	852.85	Joback Method
cpg	730.89	J/mol×K	886.35	Joback Method
cpg	748.12	J/mol×K	919.84	Joback Method

cpg	765.75	J/mol×K	953.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229673&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
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume