2«alpha»-Hydroxyamorph«alpha»-4,7(11)-diene

Other names: (-)-(1R,2S,6R,10S)-2«alpha»-Hydroxyamorpha-4,7(11)-diene
Inchi: InChI=1S/C15H24O/c1-9(2)12-6-5-11(4)15-13(12)7-10(3)8-14(15)16/h7,11,13-16H,5-6,8
InchiKey: BEIGEIPJNFKPQA-CYUUQNCZSA-N
Formula: C15H24O
SMILES: CC1=CC2C(=C(C)C)CCC(C)C2C(O)C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	53.52	kJ/mol	Joback Method
hf	-312.33	kJ/mol	Joback Method
hfus	28.55	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	666.66	K	Joback Method
tc	869.95	K	Joback Method
tf	342.63	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.39	J/mol×K	666.66	Joback Method
cpg	597.44	J/mol×K	700.54	Joback Method
cpg	615.40	J/mol×K	734.42	Joback Method
cpg	632.32	J/mol×K	768.31	Joback Method
cpg	648.22	J/mol×K	802.19	Joback Method
cpg	663.16	J/mol×K	836.07	Joback Method

cpg	677.18	J/mol×K	869.95	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=R425415&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