(-)-(1R,3R,6S,10S)-3«alpha»-Acetoxyamorpha-4,7(

Inchi: InChI=1S/C17H26O2/c1-10(2)14-7-6-11(3)15-9-17(19-13(5)18)12(4)8-16(14)15/h8,11,15
InchiKey: COZXYLPUTNJTGH-JKEMJCCQSA-N
Formula: C17H26O2
SMILES: CC(=O)OC1CC2C(C)CCC(=C(C)C)C2C=C1C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-26.74	kJ/mol	Joback Method
hf	-446.18	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	64.31	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.267		Crippen Method
mcvol	227.510	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
tb	696.53	K	Joback Method
tc	911.75	K	Joback Method
tf	376.51	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.19	J/mol×K	696.53	Joback Method
cpg	695.52	J/mol×K	732.40	Joback Method
cpg	715.53	J/mol×K	768.27	Joback Method
cpg	734.24	J/mol×K	804.14	Joback Method
cpg	751.69	J/mol×K	840.01	Joback Method
cpg	767.93	J/mol×K	875.88	Joback Method
cpg	782.98	J/mol×K	911.75	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=R515845&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