

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

Inchi:	InChI=1S/C15H24O/c1-9(2)12-6-5-10(3)13-8-15(16)11(4)7-14(12)13/h7,10,13-16H,5-6,8
InchiKey:	DMKWBQROHUFQFK-BSLXNSKLSA-N
Formula:	C15H24O
SMILES:	CC1=CC2C(=C(C)C)CCC(C)C2CC1O
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	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1666.00		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/molxK	666.66	Joback Method
cpg	597.44	J/molxK	700.54	Joback Method
cpg	615.40	J/molxK	734.42	Joback Method
cpg	632.32	J/molxK	768.31	Joback Method
cpg	648.22	J/molxK	802.19	Joback Method
cpg	663.16	J/molxK	836.07	Joback Method
cpg	677.18	J/molxK	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=R515850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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