

(-)-(1R,2S,6R,10S)-2«alpha»-Acetoxymorpha-4,7(

Inchi:	InChI=1S/C17H26O2/c1-10(2)14-7-6-12(4)17-15(14)8-11(3)9-16(17)19-13(5)18/h8,12,15
InchiKey:	CWMAZHJECLOCQL-IEAZIUSSA-N
Formula:	C17H26O2
SMILES:	CC(=O)OC1CC(C)=CC2C(=C(C)C)CCC(C)C12
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
rinpola	1800.00		NIST Webbook
rinpola	1800.00		NIST Webbook
tb	696.53	K	Joback Method
tc	911.75	K	Joback Method
tf	376.51	K	Joback Method
vc	0.862	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

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=R561501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.cheméo.com/cid/55-850-7/1R-2S-6R-10S-2-alpha-Acetoxyamorpho-4-7-11-diene.pdf>

Generated by Cheméo on 2024-04-27 09:23:51.883411083 +0000 UTC m=+16499080.803988398.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.