(+)-12-Acetoxygymnomitr-3(15)-ene

Inchi: InChI=1S/C17H26O2/c1-12-6-9-15(3)10-14(12)17(11-19-13(2)18)8-5-7-16(15,17)4/h14H
InchiKey: ZLCSCWKWOJMNOO-QBPKDAKJSA-N
Formula: C17H26O2
SMILES: C=C1CCC2(C)CC1C1(COC(C)=O)CCCC21C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	45.29	kJ/mol	Joback Method
hf	-323.31	kJ/mol	Joback Method
hfus	13.80	kJ/mol	Joback Method
hvap	59.07	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.102		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1794.00		NIST Webbook
tb	688.62	K	Joback Method
tc	916.67	K	Joback Method
tf	481.43	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.88	J/mol×K	688.62	Joback Method
cpg	682.85	J/mol×K	726.63	Joback Method
cpg	703.33	J/mol×K	764.64	Joback Method
cpg	723.72	J/mol×K	802.65	Joback Method
cpg	744.42	J/mol×K	840.65	Joback Method
cpg	765.82	J/mol×K	878.66	Joback Method
cpg	788.31	J/mol×K	916.67	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=R561289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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