(-)-15-Acetoxygymnomitr-3-ene

Inchi: InChI=1S/C17H26O2/c1-12(18)19-11-13-6-9-15(2)10-14(13)16(3)7-5-8-17(15,16)4/h6,14
InchiKey: RNPCIAPLYQGCAJ-HMQMGEFJSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC1=CCC2(C)CC1C1(C)CCCC21C
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	12.54	kJ/mol	Joback Method
hf	-361.24	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	59.87	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.102		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	693.60	K	Joback Method
tc	922.67	K	Joback Method
tf	481.03	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.58	J/mol×K	693.60	Joback Method
cpg	683.43	J/mol×K	731.78	Joback Method
cpg	703.87	J/mol×K	769.96	Joback Method
cpg	724.29	J/mol×K	808.14	Joback Method
cpg	745.09	J/mol×K	846.31	Joback Method
cpg	766.69	J/mol×K	884.49	Joback Method
cpg	789.48	J/mol×K	922.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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