4b,5«beta»-Diacetoxygymnomitr-3(15)-ene

Other names: (-)-4«beta»,5«beta»-Diacetoxygymnomitr-3(15)-ene
Inchi: InChI=1S/C19H28O4/c1-11-14-10-18(5,19(6)9-7-8-17(14,19)4)16(23-13(3)21)15(11)22-1
InchiKey: JKQYQVNQRKCWEJ-FSQANUGRSA-N
Formula: C19H28O4
SMILES: C=C1C(OC(C)=O)C(OC(C)=O)C2(C)CC1C1(C)CCCC12C
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-187.21	kJ/mol	Joback Method
hf	-650.07	kJ/mol	Joback Method
hfus	23.91	kJ/mol	Joback Method
hvap	72.06	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.642		Crippen Method
mcvol	256.570	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
tb	801.33	K	Joback Method
tc	1025.23	K	Joback Method
tf	567.65	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.61	J/mol×K	801.33	Joback Method
cpg	860.42	J/mol×K	838.65	Joback Method
cpg	883.57	J/mol×K	875.96	Joback Method
cpg	907.42	J/mol×K	913.28	Joback Method
cpg	932.30	J/mol×K	950.59	Joback Method
cpg	958.56	J/mol×K	987.91	Joback Method

cpg	986.54	J/mol×K	1025.23	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=R425995&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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