Methyl 2-epi-ziza-6(13)-en-12-oate

Inchi: InChI=1S/C16H24O2/c1-10-12-5-6-13(14(17)18-4)16(12)8-7-11(9-16)15(10,2)3/h11-13H
InchiKey: DZVKVIGAEDEAIN-JRIQMUAPSA-N
Formula: C16H24O2
SMILES: C=C1C2CCC(C(=O)OC)C23CCC(C3)C1(C)C
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	34.65	kJ/mol	Joback Method
hf	-338.25	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.568		Crippen Method
mcvol	206.860	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	1726.00		NIST Webbook
tb	660.83	K	Joback Method
tc	885.02	K	Joback Method
tf	442.02	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.62	J/mol×K	660.83	Joback Method
cpg	633.51	J/mol×K	698.19	Joback Method
cpg	653.46	J/mol×K	735.56	Joback Method
cpg	672.74	J/mol×K	772.92	Joback Method
cpg	691.62	J/mol×K	810.29	Joback Method
cpg	710.37	J/mol×K	847.65	Joback Method
cpg	729.26	J/mol×K	885.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199176&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

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