Methyl eremophila-1(10),11(13)-dien-12-oate

Inchi: InChI=1S/C16H24O2/c1-11-6-5-7-14-9-8-13(10-16(11,14)3)12(2)15(17)18-4/h7,11,13H,2
InchiKey: VCDRMAJPDHYODA-FFSVYQOJSA-N
Formula: C16H24O2
SMILES: C=C(C(=O)OC)C1CCC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	9.44	kJ/mol	Joback Method
hf	-340.56	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	59.78	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.878		Crippen Method
mcvol	213.420	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1755.00		NIST Webbook
ripol	2275.00		NIST Webbook
tb	668.60	K	Joback Method
tc	893.22	K	Joback Method
tf	381.26	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.32	J/mol×K	668.60	Joback Method
cpg	632.48	J/mol×K	706.04	Joback Method
cpg	652.47	J/mol×K	743.47	Joback Method
cpg	671.44	J/mol×K	780.91	Joback Method
cpg	689.54	J/mol×K	818.35	Joback Method
cpg	706.92	J/mol×K	855.78	Joback Method
cpg	723.73	J/mol×K	893.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R270032&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume