Methyl elema-1,4(15),11(13)-trien-12-oate

Inchi: InChI=1S/C16H24O2/c1-7-16(5)9-8-13(10-14(16)11(2)3)12(4)15(17)18-6/h7,13-14H,1-2,
InchiKey: LOTOZEIGRXLACH-SFIRGFGWSA-N
Formula: C16H24O2
SMILES: C=CC1(C)CCC(C(=C)C(=O)OC)CC1C(=C)C
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	99.88	kJ/mol	Joback Method
hf	-232.78	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	57.18	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.900		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
ripol	2149.00		NIST Webbook
ripol	2149.00		NIST Webbook
tb	642.02	K	Joback Method
tc	854.93	K	Joback Method
tf	331.84	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.86	J/mol×K	642.02	Joback Method
cpg	621.40	J/mol×K	677.50	Joback Method
cpg	640.85	J/mol×K	712.99	Joback Method
cpg	659.32	J/mol×K	748.47	Joback Method
cpg	676.92	J/mol×K	783.96	Joback Method
cpg	693.77	J/mol×K	819.44	Joback Method

cpg	709.98	J/mol×K	854.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R270027&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