Methyl (E)-eremophila-1(10),7(11)-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/h7,11H,5-6,
InchiKey: IQNNVJGAZGSJBO-LKLDIJRUSA-N
Formula: C16H24O2
SMILES: COC(=O)C(C)=C1CCC2=CCCC(C)C2(C)C1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	-25.23	kJ/mol	Joback Method
hf	-369.62	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	61.55	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.022		Crippen Method
mcvol	213.420	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1800.00		NIST Webbook
ripol	2355.00		NIST Webbook
tb	683.23	K	Joback Method
tc	909.68	K	Joback Method
tf	397.62	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.99	J/mol×K	683.23	Joback Method
cpg	630.26	J/mol×K	720.97	Joback Method
cpg	649.48	J/mol×K	758.71	Joback Method
cpg	667.81	J/mol×K	796.46	Joback Method
cpg	685.39	J/mol×K	834.20	Joback Method
cpg	702.37	J/mol×K	871.94	Joback Method
cpg	718.92	J/mol×K	909.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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