Methyl 3,7,11-trimerthyl-2,6,10-dodecatrienoate (Methyl farnesate)

Inchi: InChI=1S/C16H26O2/c1-13(2)8-6-9-14(3)10-7-11-15(4)12-16(17)18-5/h8,10,12H,6-7,9,1
InchiKey: NWKXNIPBVZQYAB-VDQVFBMKSA-N
Formula: C16H26O2
SMILES: COC(=O)C=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	64.93	kJ/mol	Joback Method
hf	-296.08	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.579		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	653.89	K	Joback Method
tc	845.23	K	Joback Method
tf	285.12	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.00	J/mol×K	653.89	Joback Method
cpg	629.22	J/mol×K	685.78	Joback Method
cpg	645.56	J/mol×K	717.67	Joback Method
cpg	661.06	J/mol×K	749.56	Joback Method
cpg	675.79	J/mol×K	781.45	Joback Method
cpg	689.78	J/mol×K	813.34	Joback Method
cpg	703.10	J/mol×K	845.23	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=R614105&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