(2E,6E)-Methyl-3,7,11-trimethyl-10-oxododecadier

Inchi: InChI=1S/C16H24O3/c1-12(2)15(17)10-9-13(3)7-6-8-14(4)11-16(18)19-5/h7,11H,1,6,8-1
InchiKey: GDSCSZUNCRRICU-FYCHQBGDSA-N
Formula: C16H24O3
SMILES: C=C(C)C(=O)CCC(C)=CCCC(C)=CC(=O)OC
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	-56.37	kJ/mol	Joback Method
hf	-400.45	kJ/mol	Joback Method
hfus	36.78	kJ/mol	Joback Method
hvap	66.60	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.758		Crippen Method
mcvol	232.410	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
tb	700.28	K	Joback Method
tc	895.05	K	Joback Method
tf	338.37	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.30	J/mol×K	700.28	Joback Method
cpg	649.07	J/mol×K	732.74	Joback Method
cpg	664.00	J/mol×K	765.20	Joback Method
cpg	678.11	J/mol×K	797.66	Joback Method
cpg	691.47	J/mol×K	830.12	Joback Method
cpg	704.12	J/mol×K	862.58	Joback Method
cpg	716.10	J/mol×K	895.05	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=R341461&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume