(9Z,12Z,15Z)-3,7-Dimethyloct-6-en-1-yl octadeca-9,12,15-trienoate

Inchi: InChI=1S/C28H48O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-28(29)30-25-24-2

InchiKey: UQLOWLBIADBCAU-QNEBEIHSSA-N

Formula: C28H48O2

SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OCCC(C)CCC=C(C)C

Mol. weight [g/mol]: 416.68

Physical Properties

Property code	Value	Unit	Source
gf	260.85	kJ/mol	Joback Method
hf	-412.24	kJ/mol	Joback Method
hfus	67.04	kJ/mol	Joback Method
hvap	86.60	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	8.892		Crippen Method
mcvol	395.620	ml/mol	McGowan Method
pc	755.15	kPa	Joback Method
rinpol	2896.10		NIST Webbook
rinpol	2896.10		NIST Webbook
tb	932.41	K	Joback Method
tc	1141.72	K	Joback Method
tf	428.20	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.01	J/mol×K	932.41	Joback Method
cpg	1329.80	J/mol×K	967.30	Joback Method
cpg	1350.61	J/mol×K	1002.18	Joback Method
cpg	1370.54	J/mol×K	1037.07	Joback Method
cpg	1389.70	J/mol×K	1071.95	Joback Method
cpg	1408.22	J/mol×K	1106.84	Joback Method
cpg	1426.20	J/mol×K	1141.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412989&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume