(9Z,12Z)-(E)-3,7-Dimethylocta-2,6-dien-1-yl octadeca-9,12-dienoate

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: SDVRIIKZIMWDSJ-BUWFTCIHSA-N

Formula: C28H48O2

SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C

Mol. weight [g/mol]: 416.68

Physical Properties

Property code	Value	Unit	Source
gf	254.74	kJ/mol	Joback Method
hf	-416.75	kJ/mol	Joback Method
hfus	69.25	kJ/mol	Joback Method
hvap	87.07	kJ/mol	Joback Method
log10ws	-9.82		Crippen Method
logp	9.036		Crippen Method
mcvol	395.620	ml/mol	McGowan Method
pc	753.91	kPa	Joback Method
rinpol	2923.80		NIST Webbook
rinpol	2923.80		NIST Webbook
tb	932.73	K	Joback Method
tc	1142.16	K	Joback Method
tf	429.24	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.25	J/mol×K	932.73	Joback Method
cpg	1329.12	J/mol×K	967.63	Joback Method
cpg	1350.02	J/mol×K	1002.54	Joback Method
cpg	1370.05	J/mol×K	1037.44	Joback Method
cpg	1389.35	J/mol×K	1072.35	Joback Method
cpg	1408.01	J/mol×K	1107.25	Joback Method
cpg	1426.17	J/mol×K	1142.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412990&Units=SI

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