(9Z,12Z,15Z)-(E)-3,7-Dimethylocta-2,6-dien-1-yl octadeca-9,12,15-trienoate

Inchi: InChI=1S/C28H46O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-28(29)30-25-24-2
InchiKey: XGCMITBQDORUDF-ZKYCGLNMSA-N
Formula: C28H46O2
SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 414.66

Physical Properties

Property code	Value	Unit	Source
gf	334.96	kJ/mol	Joback Method
hf	-299.53	kJ/mol	Joback Method
hfus	69.45	kJ/mol	Joback Method
hvap	87.03	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.812		Crippen Method
mcvol	391.320	ml/mol	McGowan Method
pc	775.91	kPa	Joback Method
rinpol	2934.10		NIST Webbook
rinpol	2934.10		NIST Webbook
tb	936.89	K	Joback Method
tc	1147.02	K	Joback Method
tf	424.16	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1279.89	J/mol×K	936.89	Joback Method
cpg	1301.35	J/mol×K	971.91	Joback Method
cpg	1321.96	J/mol×K	1006.93	Joback Method
cpg	1341.88	J/mol×K	1041.95	Joback Method
cpg	1361.22	J/mol×K	1076.98	Joback Method
cpg	1380.12	J/mol×K	1112.00	Joback Method
cpg	1398.70	J/mol×K	1147.02	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=U412978&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