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

Inchi: InChI=1S/C28H50O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-28(29)30-25-24-2
InchiKey: RHFFIMUAJDREAJ-UTJQPWESSA-N
Formula: C28H50O2
SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 418.70

Physical Properties

Property code	Value	Unit	Source
gf	180.63	kJ/mol	Joback Method
hf	-529.46	kJ/mol	Joback Method
hfus	66.84	kJ/mol	Joback Method
hvap	86.64	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	9.116		Crippen Method
mcvol	399.920	ml/mol	McGowan Method
pc	734.03	kPa	Joback Method
rinpol	2887.80		NIST Webbook
rinpol	2887.80		NIST Webbook
tb	928.25	K	Joback Method
tc	1137.22	K	Joback Method
tf	433.28	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1335.25	J/mol×K	928.25	Joback Method
cpg	1357.53	J/mol×K	963.08	Joback Method
cpg	1378.68	J/mol×K	997.91	Joback Method
cpg	1398.80	J/mol×K	1032.74	Joback Method
cpg	1418.00	J/mol×K	1067.56	Joback Method
cpg	1436.36	J/mol×K	1102.39	Joback Method
cpg	1454.01	J/mol×K	1137.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412988&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