(2E,6E)-3,7,11-Trimethyldodeca-2,6,10-trien-1-yl stearate

Inchi: InChI=1S/C33H60O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-27-33(34)35-29-28-
InchiKey: YQPQEVWUUVTRQA-XPYMXISMSA-N
Formula: C33H60O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 488.83
CAS: 69624-82-4

Physical Properties

Property code	Value	Unit	Source
gf	208.07	kJ/mol	Joback Method
hf	-646.96	kJ/mol	Joback Method
hfus	80.69	kJ/mol	Joback Method
hvap	98.32	kJ/mol	Joback Method
log10ws	-12.06		Crippen Method
logp	11.210		Crippen Method
mcvol	470.370	ml/mol	McGowan Method
pc	575.36	kPa	Joback Method
rinpol	3446.50		NIST Webbook
rinpol	3446.50		NIST Webbook
tb	1042.85	K	Joback Method
tc	1297.20	K	Joback Method
tf	476.71	K	Joback Method
vc	1.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1666.03	J/mol×K	1042.85	Joback Method
cpg	1693.36	J/mol×K	1085.24	Joback Method
cpg	1719.29	J/mol×K	1127.63	Joback Method
cpg	1744.06	J/mol×K	1170.02	Joback Method
cpg	1767.87	J/mol×K	1212.42	Joback Method
cpg	1790.93	J/mol×K	1254.81	Joback Method
cpg	1813.45	J/mol×K	1297.20	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=C69624824&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