3,7,11-trimethyldodeca-2,6,10-trien-1-yl palmitate

Inchi: InChI=1S/C31H56O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-25-31(32)33-27-26-30(5)2
InchiKey: JXOGISMTOCGSHX-GDHXXOHCSA-N
Formula: C31H56O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 460.78
CAS: 157501-12-7

Physical Properties

Property code	Value	Unit	Source
gf	191.23	kJ/mol	Joback Method
hf	-605.68	kJ/mol	Joback Method
hfus	75.51	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-11.22		Crippen Method
logp	10.430		Crippen Method
mcvol	442.190	ml/mol	McGowan Method
pc	632.25	kPa	Joback Method
rinpol	3204.10		NIST Webbook
rinpol	3204.10		NIST Webbook
tb	997.09	K	Joback Method
tc	1229.34	K	Joback Method
tf	454.17	K	Joback Method
vc	1.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1531.69	J/mol×K	997.09	Joback Method
cpg	1556.64	J/mol×K	1035.80	Joback Method
cpg	1580.33	J/mol×K	1074.51	Joback Method
cpg	1602.92	J/mol×K	1113.22	Joback Method
cpg	1624.56	J/mol×K	1151.93	Joback Method
cpg	1645.40	J/mol×K	1190.63	Joback Method
cpg	1665.60	J/mol×K	1229.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C157501127&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

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