(E)-3,7-Dimethylocta-2,6-dien-1-yl palmitate

Inchi: InChI=1S/C26H48O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26(27)28-23-22-25(4)20
InchiKey: CRFQQFDSKWNZIZ-YYDJUVGSSA-N
Formula: C26H48O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 392.66
CAS: 3681-73-0

Physical Properties

Property code	Value	Unit	Source
gf	77.46	kJ/mol	Joback Method
hf	-609.91	kJ/mol	Joback Method
hfus	63.67	kJ/mol	Joback Method
hvap	82.70	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	8.704		Crippen Method
mcvol	376.040	ml/mol	McGowan Method
pc	791.71	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	878.65	K	Joback Method
tc	1075.71	K	Joback Method
tf	416.86	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1232.21	J/mol×K	878.65	Joback Method
cpg	1253.79	J/mol×K	911.49	Joback Method
cpg	1274.23	J/mol×K	944.34	Joback Method
cpg	1293.62	J/mol×K	977.18	Joback Method
cpg	1312.02	J/mol×K	1010.03	Joback Method
cpg	1329.51	J/mol×K	1042.87	Joback Method
cpg	1346.15	J/mol×K	1075.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3681730&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