3,7-Dimethyloct-6-en-1-yl palmitate

Inchi: InChI=1S/C26H50O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26(27)28-23-22-25(4)20
InchiKey: YTGIONGRGTWTNY-UHFFFAOYSA-N
Formula: C26H50O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 394.67
CAS: 7243-93-8

Physical Properties

Property code	Value	Unit	Source
gf	3.35	kJ/mol	Joback Method
hf	-722.62	kJ/mol	Joback Method
hfus	61.25	kJ/mol	Joback Method
hvap	82.28	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	8.784		Crippen Method
mcvol	380.340	ml/mol	McGowan Method
pc	770.32	kPa	Joback Method
rinpol	2713.80		NIST Webbook
rinpol	2713.80		NIST Webbook
tb	874.17	K	Joback Method
tc	1070.36	K	Joback Method
tf	420.90	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1259.28	J/mol×K	874.17	Joback Method
cpg	1281.42	J/mol×K	906.87	Joback Method
cpg	1302.33	J/mol×K	939.57	Joback Method
cpg	1322.05	J/mol×K	972.26	Joback Method
cpg	1340.65	J/mol×K	1004.96	Joback Method
cpg	1358.19	J/mol×K	1037.66	Joback Method
cpg	1374.72	J/mol×K	1070.36	Joback Method

Sources

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=C7243938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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