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

Inchi: InChI=1S/C28H52O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-28(29)30-25-24-2
InchiKey: ILBHDXCOZDEXGP-SOYKGTTHSA-N
Formula: C28H52O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 420.71
CAS: 28219-83-2

Physical Properties

Property code	Value	Unit	Source
gf	94.30	kJ/mol	Joback Method
hf	-651.19	kJ/mol	Joback Method
hfus	68.85	kJ/mol	Joback Method
hvap	87.15	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	9.484		Crippen Method
mcvol	404.220	ml/mol	McGowan Method
pc	712.63	kPa	Joback Method
rinpol	2951.10		NIST Webbook
rinpol	2951.10		NIST Webbook
tb	924.41	K	Joback Method
tc	1133.64	K	Joback Method
tf	439.40	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1361.61	J/mol×K	924.41	Joback Method
cpg	1384.52	J/mol×K	959.28	Joback Method
cpg	1406.17	J/mol×K	994.15	Joback Method
cpg	1426.67	J/mol×K	1029.02	Joback Method
cpg	1446.09	J/mol×K	1063.89	Joback Method
cpg	1464.52	J/mol×K	1098.77	Joback Method
cpg	1482.07	J/mol×K	1133.64	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=C28219832&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

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