3,7-dimethyloct-6-en-1-yl stearate

Inchi: InChI=1S/C28H54O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-28(29)30-25-24-2
InchiKey: UTULGKGDQRRQHR-UHFFFAOYSA-N
Formula: C28H54O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 422.73
CAS: 28228-30-0

Physical Properties

Property code	Value	Unit	Source
gf	20.19	kJ/mol	Joback Method
hf	-763.90	kJ/mol	Joback Method
hfus	66.43	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	-10.02		Crippen Method
logp	9.564		Crippen Method
mcvol	408.520	ml/mol	McGowan Method
pc	694.35	kPa	Joback Method
rinpol	2915.20		NIST Webbook
rinpol	2915.20		NIST Webbook
tb	919.93	K	Joback Method
tc	1129.40	K	Joback Method
tf	443.44	K	Joback Method
vc	1.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1389.34	J/mol×K	919.93	Joback Method
cpg	1412.81	J/mol×K	954.84	Joback Method
cpg	1434.86	J/mol×K	989.75	Joback Method
cpg	1455.58	J/mol×K	1024.66	Joback Method
cpg	1475.04	J/mol×K	1059.58	Joback Method
cpg	1493.32	J/mol×K	1094.49	Joback Method
cpg	1510.51	J/mol×K	1129.40	Joback Method

Sources

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=C28228300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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