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

Inchi: InChI=1S/C19H36O2/c1-5-6-7-8-9-10-14-19(20)21-16-15-18(4)13-11-12-17(2)3/h12,18H
InchiKey: ULWMBBYWQZNAMT-UHFFFAOYSA-N
Formula: C19H36O2
SMILES: CCCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 296.49
CAS: 72934-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-55.59	kJ/mol	Joback Method
hf	-578.14	kJ/mol	Joback Method
hfus	43.12	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	6.053		Crippen Method
mcvol	281.710	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2015.90		NIST Webbook
rinpol	2015.90		NIST Webbook
tb	714.01	K	Joback Method
tc	890.48	K	Joback Method
tf	342.01	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.29	J/mol×K	714.01	Joback Method
cpg	845.37	J/mol×K	743.42	Joback Method
cpg	863.55	J/mol×K	772.83	Joback Method
cpg	880.86	J/mol×K	802.25	Joback Method
cpg	897.32	J/mol×K	831.66	Joback Method
cpg	912.96	J/mol×K	861.07	Joback Method
cpg	927.82	J/mol×K	890.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72934180&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