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

Inchi: InChI=1S/C22H42O2/c1-5-6-7-8-9-10-11-12-13-17-22(23)24-19-18-21(4)16-14-15-20(2)3
InchiKey: GARTVHIDFKCTCG-UHFFFAOYSA-N
Formula: C22H42O2
SMILES: CCCCCCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 338.57
CAS: 72934-07-7

Physical Properties

Property code	Value	Unit	Source
gf	-30.33	kJ/mol	Joback Method
hf	-640.06	kJ/mol	Joback Method
hfus	50.89	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	7.223		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook
tb	782.65	K	Joback Method
tc	963.27	K	Joback Method
tf	375.82	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.90	J/mol×K	782.65	Joback Method
cpg	1027.10	J/mol×K	812.75	Joback Method
cpg	1046.29	J/mol×K	842.86	Joback Method
cpg	1064.51	J/mol×K	872.96	Joback Method
cpg	1081.79	J/mol×K	903.07	Joback Method
cpg	1098.17	J/mol×K	933.17	Joback Method
cpg	1113.70	J/mol×K	963.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72934077&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

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