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

Inchi: InChI=1S/C22H40O2/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: LNEUQAMNTXRCPI-DYTRJAOYSA-N

Formula: C22H40O2

SMILES: CCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)C

Mol. weight [g/mol]: 336.55

CAS: 72934-09-9

Physical Properties

Property code	Value	Unit	Source
gf	43.78	kJ/mol	Joback Method
hf	-527.35	kJ/mol	Joback Method
hfus	53.31	kJ/mol	Joback Method
hvap	73.80	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.143		Crippen Method
mcvol	319.680	ml/mol	McGowan Method
pc	995.13	kPa	Joback Method
rinpol	2349.00		NIST Webbook
tb	787.13	K	Joback Method
tc	970.60	K	Joback Method
tf	371.78	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.68	J/mol×K	787.13	Joback Method
cpg	1001.33	J/mol×K	817.71	Joback Method
cpg	1020.02	J/mol×K	848.29	Joback Method
cpg	1037.79	J/mol×K	878.87	Joback Method
cpg	1054.69	J/mol×K	909.45	Joback Method
cpg	1070.78	J/mol×K	940.02	Joback Method
cpg	1086.10	J/mol×K	970.60	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=C72934099&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