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

Inchi: InChI=1S/C24H44O2/c1-5-6-7-8-9-10-11-12-13-14-15-19-24(25)26-21-20-23(4)18-16-17
InchiKey: BVBISCLEXKZRHD-BSYVCWPDSA-N
Formula: C24H44O2
SMILES: CCCCCCCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 364.61
CAS: 72934-10-2

Physical Properties

Property code	Value	Unit	Source
gf	60.62	kJ/mol	Joback Method
hf	-568.63	kJ/mol	Joback Method
hfus	58.49	kJ/mol	Joback Method
hvap	78.25	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	7.923		Crippen Method
mcvol	347.860	ml/mol	McGowan Method
pc	884.72	kPa	Joback Method
rinpol	2548.20		NIST Webbook
rinpol	2548.20		NIST Webbook
tb	832.89	K	Joback Method
tc	1021.55	K	Joback Method
tf	394.32	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1105.43	J/mol×K	832.89	Joback Method
cpg	1125.95	J/mol×K	864.33	Joback Method
cpg	1145.43	J/mol×K	895.78	Joback Method
cpg	1163.93	J/mol×K	927.22	Joback Method
cpg	1181.51	J/mol×K	958.67	Joback Method
cpg	1198.23	J/mol×K	990.11	Joback Method
cpg	1214.15	J/mol×K	1021.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72934102&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

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