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

Inchi: InChI=1S/C20H36O2/c1-5-6-7-8-9-10-11-15-20(21)22-17-16-19(4)14-12-13-18(2)3/h13,1
InchiKey: ICAWXCQTUNYABR-KNTRCKAVSA-N
Formula: C20H36O2
SMILES: CCCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 308.50
CAS: 10471-94-0

Physical Properties

Property code	Value	Unit	Source
gf	26.94	kJ/mol	Joback Method
hf	-486.07	kJ/mol	Joback Method
hfus	48.13	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.363		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
rinpol	2151.30		NIST Webbook
rinpol	2151.30		NIST Webbook
tb	741.37	K	Joback Method
tc	922.37	K	Joback Method
tf	349.24	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.42	J/mol×K	741.37	Joback Method
cpg	880.33	J/mol×K	771.54	Joback Method
cpg	898.33	J/mol×K	801.70	Joback Method
cpg	915.45	J/mol×K	831.87	Joback Method
cpg	931.75	J/mol×K	862.04	Joback Method
cpg	947.27	J/mol×K	892.21	Joback Method
cpg	962.05	J/mol×K	922.37	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=C10471940&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