3,7-dimethyl-6-octenyl 3,7-dimethyloct-6-enoate

Other names: 3,7-Dimethyloct-6-en-1-yl 3,7-dimethyloct-6-enoate
Inchi: InChI=1S/C20H36O2/c1-16(2)9-7-11-18(5)13-14-22-20(21)15-19(6)12-8-10-17(3)4/h9-10
InchiKey: HUZXZYWMBWQTNX-UHFFFAOYSA-N
Formula: C20H36O2
SMILES: CC(C)=CCCC(C)CCOC(=O)CC(C)CCC=C(C)C
Mol. weight [g/mol]: 308.50
CAS: 82766-40-3

Physical Properties

Property code	Value	Unit	Source
gf	22.06	kJ/mol	Joback Method
hf	-496.63	kJ/mol	Joback Method
hfus	41.08	kJ/mol	Joback Method
hvap	68.57	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.075		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	2047.40		NIST Webbook
rinpol	2047.40		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	740.49	K	Joback Method
tc	925.36	K	Joback Method
tf	319.24	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.34	J/mol×K	740.49	Joback Method
cpg	881.69	J/mol×K	771.30	Joback Method
cpg	900.06	J/mol×K	802.11	Joback Method
cpg	917.52	J/mol×K	832.93	Joback Method

cpg	934.09	J/mol×K	863.74	Joback Method
cpg	949.83	J/mol×K	894.55	Joback Method
cpg	964.79	J/mol×K	925.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82766403&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