3,7-Dimethyloct-6-en-1-yl 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]: 308.51

Physical Properties

Property code	Value	Unit	Source
hf	-666.46	kJ/mol	Cheméo Relay (1.0)
hfus	41.08	kJ/mol	Joback Method
hvap	86.58	kJ/mol	Cheméo Relay (1.0)
logp	6.075		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
rinpol	2032.00		NIST Webbook
rinpol	2047.40		NIST Webbook
rinpol	2047.40		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	579.59	K	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82766403&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature