3,7-Dimethyloct-6-en-1-yl decanoate

Inchi: InChI=1S/C20H38O2/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: XQIVXZXBZSEVKC-UHFFFAOYSA-N
Formula: C20H38O2
SMILES: CCCCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 310.51
CAS: 72934-06-6

Physical Properties

Property code	Value	Unit	Source
gf	-47.17	kJ/mol	Joback Method
hf	-598.78	kJ/mol	Joback Method
hfus	45.71	kJ/mol	Joback Method
hvap	68.92	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.443		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2113.60		NIST Webbook
rinpol	2113.60		NIST Webbook
tb	736.89	K	Joback Method
tc	914.15	K	Joback Method
tf	353.28	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.53	J/mol×K	736.89	Joback Method
cpg	904.98	J/mol×K	766.43	Joback Method
cpg	923.48	J/mol×K	795.98	Joback Method
cpg	941.09	J/mol×K	825.52	Joback Method
cpg	957.82	J/mol×K	855.06	Joback Method
cpg	973.71	J/mol×K	884.61	Joback Method
cpg	988.79	J/mol×K	914.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72934066&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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