Succinic acid, di(3,7-dimethyloct-6-en-1-yl) ester

Inchi: InChI=1S/C24H42O4/c1-19(2)9-7-11-21(5)15-17-27-23(25)13-14-24(26)28-18-16-22(6)12-8-10-20(3)4/h9-10,21-22H,7-8,11-18H2,1-6H3

InchiKey: GMLQUIFZFBXXCI-UHFFFAOYSA-N

Formula: C24H42O4

SMILES: CC(C)=CCCC(C)CCOC(=O)CCC(=O)OCCC(C)CCC=C(C)C

Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-178.18	kJ/mol	Joback Method
hf	-823.99	kJ/mol	Joback Method
hfus	54.23	kJ/mol	Joback Method
hvap	86.63	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.398		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	918.27	kPa	Joback Method
rinpol	2619.00		NIST Webbook
tb	908.30	K	Joback Method
tc	1112.42	K	Joback Method
tf	436.48	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.46	J/mol×K	908.30	Joback Method
cpg	1182.43	J/mol×K	942.32	Joback Method
cpg	1200.22	J/mol×K	976.34	Joback Method
cpg	1216.88	J/mol×K	1010.36	Joback Method
cpg	1232.48	J/mol×K	1044.38	Joback Method
cpg	1247.06	J/mol×K	1078.40	Joback Method
cpg	1260.70	J/mol×K	1112.42	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=U353352&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