Succinic acid, 3,7-dimethyloct-6-en-1-yl octyl ester

Inchi: InChI=1S/C22H40O4/c1-5-6-7-8-9-10-17-25-21(23)14-15-22(24)26-18-16-20(4)13-11-12

InchiKey: BVPJRJVVWOPAFK-UHFFFAOYSA-N

Formula: C22H40O4

SMILES: CCCCCCCCOC(=O)CCC(=O)OCCC(C)CCC=C(C)C

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-264.25	kJ/mol	Joback Method
hf	-884.86	kJ/mol	Joback Method
hfus	53.68	kJ/mol	Joback Method
hvap	82.53	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.986		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	993.25	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	858.94	K	Joback Method
tc	1052.73	K	Joback Method
tf	447.98	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.90	J/mol×K	858.94	Joback Method
cpg	1084.51	J/mol×K	891.24	Joback Method
cpg	1101.99	J/mol×K	923.54	Joback Method
cpg	1118.37	J/mol×K	955.83	Joback Method
cpg	1133.69	J/mol×K	988.13	Joback Method
cpg	1147.97	J/mol×K	1020.43	Joback Method
cpg	1161.26	J/mol×K	1052.73	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=U353342&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