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

Inchi: InChI=1S/C20H36O4/c1-16(2)8-6-10-18(5)13-15-24-20(22)12-11-19(21)23-14-7-9-17(3)4

InchiKey: UGQGVLOOSRYMCZ-UHFFFAOYSA-N

Formula: C20H36O4

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

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-283.53	kJ/mol	Joback Method
hf	-848.86	kJ/mol	Joback Method
hfus	44.98	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	5.062		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	812.74	K	Joback Method
tc	1001.90	K	Joback Method
tf	410.44	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.47	J/mol×K	812.74	Joback Method
cpg	962.43	J/mol×K	844.27	Joback Method
cpg	979.35	J/mol×K	875.79	Joback Method
cpg	995.26	J/mol×K	907.32	Joback Method
cpg	1010.18	J/mol×K	938.85	Joback Method
cpg	1024.14	J/mol×K	970.38	Joback Method
cpg	1037.17	J/mol×K	1001.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353339&Units=SI

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