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

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

InchiKey: JSPKYCAAPZCHEZ-UHFFFAOYSA-N

Formula: C20H36O4

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

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-281.09	kJ/mol	Joback Method
hf	-843.58	kJ/mol	Joback Method
hfus	48.50	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	5.206		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	2275.00		NIST Webbook
tb	813.18	K	Joback Method
tc	1001.16	K	Joback Method
tf	425.44	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.98	J/mol×K	813.18	Joback Method
cpg	961.83	J/mol×K	844.51	Joback Method
cpg	978.66	J/mol×K	875.84	Joback Method
cpg	994.50	J/mol×K	907.17	Joback Method
cpg	1009.38	J/mol×K	938.50	Joback Method
cpg	1023.31	J/mol×K	969.83	Joback Method
cpg	1036.34	J/mol×K	1001.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353340&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

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