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

Inchi: InChI=1S/C30H56O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-25-33-29(31)22-23-30(3

InchiKey: IIFRFNXLJOVISE-UHFFFAOYSA-N

Formula: C30H56O4

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

Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-196.89	kJ/mol	Joback Method
hf	-1049.98	kJ/mol	Joback Method
hfus	74.40	kJ/mol	Joback Method
hvap	100.34	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	9.107		Crippen Method
mcvol	444.140	ml/mol	McGowan Method
pc	643.85	kPa	Joback Method
rinpol	3265.00		NIST Webbook
rinpol	3265.00		NIST Webbook
tb	1041.98	K	Joback Method
tc	1299.12	K	Joback Method
tf	538.14	K	Joback Method
vc	1.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1576.77	J/mol×K	1041.98	Joback Method
cpg	1600.08	J/mol×K	1084.84	Joback Method
cpg	1621.31	J/mol×K	1127.69	Joback Method
cpg	1640.56	J/mol×K	1170.55	Joback Method
cpg	1657.97	J/mol×K	1213.40	Joback Method
cpg	1673.67	J/mol×K	1256.26	Joback Method
cpg	1687.78	J/mol×K	1299.12	Joback Method

Sources

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=U353349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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