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

Inchi: InChI=1S/C32H60O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-27-35-31(33)24-2

InchiKey: DLFGZWOZDSIRIM-UHFFFAOYSA-N

Formula: C32H60O4

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

Mol. weight [g/mol]: 508.82

Physical Properties

Property code	Value	Unit	Source
gf	-180.05	kJ/mol	Joback Method
hf	-1091.26	kJ/mol	Joback Method
hfus	79.58	kJ/mol	Joback Method
hvap	104.79	kJ/mol	Joback Method
log10ws	-10.55		Crippen Method
logp	9.887		Crippen Method
mcvol	472.320	ml/mol	McGowan Method
pc	585.42	kPa	Joback Method
rinpol	3467.00		NIST Webbook
rinpol	3467.00		NIST Webbook
tb	1087.74	K	Joback Method
tc	1374.34	K	Joback Method
tf	560.68	K	Joback Method
vc	1.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1708.34	J/mol×K	1087.74	Joback Method
cpg	1733.45	J/mol×K	1135.51	Joback Method
cpg	1756.02	J/mol×K	1183.27	Joback Method
cpg	1776.23	J/mol×K	1231.04	Joback Method
cpg	1794.29	J/mol×K	1278.81	Joback Method
cpg	1810.38	J/mol×K	1326.58	Joback Method
cpg	1824.68	J/mol×K	1374.34	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=U353351&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