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

Inchi: InChI=1S/C31H58O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-26-34-30(32)23-24-3

InchiKey: FFMPJYWZEHSRPH-UHFFFAOYSA-N

Formula: C31H58O4

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

Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
gf	-188.47	kJ/mol	Joback Method
hf	-1070.62	kJ/mol	Joback Method
hfus	76.99	kJ/mol	Joback Method
hvap	102.56	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	9.497		Crippen Method
mcvol	458.230	ml/mol	McGowan Method
pc	613.60	kPa	Joback Method
rinpol	3366.00		NIST Webbook
rinpol	3366.00		NIST Webbook
tb	1064.86	K	Joback Method
tc	1335.88	K	Joback Method
tf	549.41	K	Joback Method
vc	1.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1642.42	J/mol×K	1064.86	Joback Method
cpg	1666.59	J/mol×K	1110.03	Joback Method
cpg	1688.47	J/mol×K	1155.20	Joback Method
cpg	1708.19	J/mol×K	1200.37	Joback Method
cpg	1725.92	J/mol×K	1245.54	Joback Method
cpg	1741.81	J/mol×K	1290.71	Joback Method
cpg	1756.01	J/mol×K	1335.88	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=U353350&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

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