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

Inchi: InChI=1S/C29H54O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-24-32-28(30)21-22-29(31)3

InchiKey: VNNAPXSMRPBWQF-UHFFFAOYSA-N

Formula: C29H54O4

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

Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-205.31	kJ/mol	Joback Method
hf	-1029.34	kJ/mol	Joback Method
hfus	71.81	kJ/mol	Joback Method
hvap	98.11	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	8.717		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	676.41	kPa	Joback Method
rinpol	3164.00		NIST Webbook
tb	1019.10	K	Joback Method
tc	1263.92	K	Joback Method
tf	526.87	K	Joback Method
vc	1.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.42	J/mol×K	1019.10	Joback Method
cpg	1533.94	J/mol×K	1059.90	Joback Method
cpg	1554.56	J/mol×K	1100.71	Joback Method
cpg	1573.37	J/mol×K	1141.51	Joback Method
cpg	1590.49	J/mol×K	1182.31	Joback Method
cpg	1606.00	J/mol×K	1223.12	Joback Method
cpg	1620.02	J/mol×K	1263.92	Joback Method

Sources

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=U353348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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