Succinic acid, 3-methylbut-3-enyl octadecyl ester

Inchi: InChI=1S/C27H50O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-30-26(28)20-21

InchiKey: CKVLEHZLHBWGNY-UHFFFAOYSA-N

Formula: C27H50O4

SMILES: C=C(C)CCOC(=O)CCC(=O)OCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-212.09	kJ/mol	Joback Method
hf	-974.57	kJ/mol	Joback Method
hfus	68.67	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.081		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	742.05	kPa	Joback Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook
tb	966.30	K	Joback Method
tc	1191.27	K	Joback Method
tf	522.65	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.32	J/mol×K	966.30	Joback Method
cpg	1400.62	J/mol×K	1003.79	Joback Method
cpg	1420.22	J/mol×K	1041.29	Joback Method
cpg	1438.18	J/mol×K	1078.78	Joback Method
cpg	1454.57	J/mol×K	1116.28	Joback Method
cpg	1469.46	J/mol×K	1153.77	Joback Method
cpg	1482.91	J/mol×K	1191.27	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=U353454&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

Latest version available from:
https://www.chemeo.com/cid/67-824-3/Succinic-acid-3-methylbut-3-enyl-octadecyl-ester.pdf
Generated by Cheméo on 2024-04-26 18:03:41.620391639 +0000 UTC m=+16443870.540968951.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.