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

Inchi: InChI=1S/C29H54O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-25-32-28(30)22-19
InchiKey: NLTYUYKYLIXUSJ-UHFFFAOYSA-N
Formula: C29H54O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-195.25	kJ/mol	Joback Method
hf	-1015.85	kJ/mol	Joback Method
hfus	73.85	kJ/mol	Joback Method
hvap	97.87	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.861		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	670.12	kPa	Joback Method
rinpol	3235.00		NIST Webbook
tb	1012.06	K	Joback Method
tc	1258.72	K	Joback Method
tf	545.19	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1508.79	J/mol×K	1012.06	Joback Method
cpg	1531.49	J/mol×K	1053.17	Joback Method
cpg	1552.14	J/mol×K	1094.28	Joback Method
cpg	1570.83	J/mol×K	1135.39	Joback Method
cpg	1587.66	J/mol×K	1176.50	Joback Method
cpg	1602.71	J/mol×K	1217.61	Joback Method
cpg	1616.09	J/mol×K	1258.72	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=U354041&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