Adipic acid, octadecyl pent-4-enyl ester

Inchi: InChI=1S/C29H54O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-23-27-33-29(31)25-2
InchiKey: FICQPOWOLLKCRD-UHFFFAOYSA-N
Formula: C29H54O4
SMILES: C=CCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-186.70	kJ/mol	Joback Method
hf	-1006.06	kJ/mol	Joback Method
hfus	75.16	kJ/mol	Joback Method
hvap	97.79	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.861		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	668.39	kPa	Joback Method
rinpol	3230.00		NIST Webbook
rinpol	3230.00		NIST Webbook
tb	1012.18	K	Joback Method
tc	1261.06	K	Joback Method
tf	559.15	K	Joback Method
vc	1.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1509.12	J/mol×K	1012.18	Joback Method
cpg	1603.33	J/mol×K	1219.58	Joback Method
cpg	1588.31	J/mol×K	1178.10	Joback Method
cpg	1571.47	J/mol×K	1136.62	Joback Method
cpg	1552.72	J/mol×K	1095.14	Joback Method
cpg	1531.97	J/mol×K	1053.66	Joback Method
cpg	1616.64	J/mol×K	1261.06	Joback Method
dvisc	0.0000146	Pa×s	1012.18	Joback Method

dvisc	0.0000196	Pa×s	936.68	Joback Method
dvisc	0.0000277	Pa×s	861.17	Joback Method
dvisc	0.0000420	Pa×s	785.67	Joback Method
dvisc	0.0000693	Pa×s	710.16	Joback Method
dvisc	0.0001291	Pa×s	634.66	Joback Method
dvisc	0.0002845	Pa×s	559.15	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=U353807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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