Adipic acid, cis-hex-3-enyl heptadecyl ester

Inchi: InChI=1S/C29H54O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-23-27-33-29(31)25-21-
InchiKey: HVGZSWXSJBLGNE-VURMDHGXSA-N
Formula: C29H54O4
SMILES: CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-194.32	kJ/mol	Joback Method
hf	-1014.27	kJ/mol	Joback Method
hfus	76.64	kJ/mol	Joback Method
hvap	98.42	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.861		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	671.85	kPa	Joback Method
rinpol	3250.00		NIST Webbook
tb	1019.66	K	Joback Method
tc	1269.19	K	Joback Method
tf	555.83	K	Joback Method
vc	1.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.50	J/mol×K	1019.66	Joback Method
cpg	1607.70	J/mol×K	1227.60	Joback Method
cpg	1591.97	J/mol×K	1186.01	Joback Method
cpg	1574.59	J/mol×K	1144.42	Joback Method
cpg	1555.46	J/mol×K	1102.84	Joback Method
cpg	1534.47	J/mol×K	1061.25	Joback Method
cpg	1621.89	J/mol×K	1269.19	Joback Method
dvisc	0.0000118	Pa×s	1019.66	Joback Method
dvisc	0.0000160	Pa×s	942.36	Joback Method

dvisc	0.0000228	Pa×s	865.05	Joback Method
dvisc	0.0000349	Pa×s	787.74	Joback Method
dvisc	0.0000587	Pa×s	710.44	Joback Method
dvisc	0.0001119	Pa×s	633.13	Joback Method
dvisc	0.0002552	Pa×s	555.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353985&Units=SI
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

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

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