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

Inchi: InChI=1S/C27H50O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-21-25-31-27(29)23-19-18-22-
InchiKey: UJPOWTRPAIUPAO-VURMDHGXSA-N
Formula: C27H50O4
SMILES: CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-211.16	kJ/mol	Joback Method
hf	-972.99	kJ/mol	Joback Method
hfus	71.46	kJ/mol	Joback Method
hvap	93.97	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.081		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	744.07	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	973.90	K	Joback Method
tc	1201.27	K	Joback Method
tf	533.29	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.80	J/mol×K	973.90	Joback Method
cpg	1403.23	J/mol×K	1011.80	Joback Method
cpg	1423.02	J/mol×K	1049.69	Joback Method
cpg	1441.24	J/mol×K	1087.59	Joback Method
cpg	1457.97	J/mol×K	1125.48	Joback Method
cpg	1473.28	J/mol×K	1163.38	Joback Method
cpg	1487.25	J/mol×K	1201.27	Joback Method
dvisc	0.0003337	Pa×s	533.29	Joback Method

dvisc	0.0001486	Pa×s	606.72	Joback Method
dvisc	0.0000788	Pa×s	680.16	Joback Method
dvisc	0.0000473	Pa×s	753.60	Joback Method
dvisc	0.0000310	Pa×s	827.03	Joback Method
dvisc	0.0000218	Pa×s	900.46	Joback Method
dvisc	0.0000162	Pa×s	973.90	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=U353983&Units=SI

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