

Adipic acid, cis-non-3-enyl tetradecyl ester

Inchi: InChI=1S/C29H54O4/c1-3-5-7-9-11-12-13-14-15-17-19-23-27-33-29(31)25-21-20-24-28(30)22-26
InchiKey: FYXXZJWYBSRZJQ-VLGSPTGOSA-N
Formula: C29H54O4
SMILES: CCCCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCC
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	3225.00		NIST Webbook
rinpol	3225.00		NIST Webbook
tb	1019.66	K	Joback Method
tc	1269.19	K	Joback Method
tf	555.83	K	Joback Method
vc	1.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.50	J/molxK	1019.66	Joback Method
cpg	1534.47	J/molxK	1061.25	Joback Method
cpg	1555.46	J/molxK	1102.84	Joback Method
cpg	1574.59	J/molxK	1144.42	Joback Method
cpg	1591.97	J/molxK	1186.01	Joback Method
cpg	1607.70	J/molxK	1227.60	Joback Method
cpg	1621.89	J/molxK	1269.19	Joback Method
dvisc	0.0002552	Paxs	555.83	Joback Method

dvisc	0.0001119	Paxs	633.13	Joback Method
dvisc	0.0000587	Paxs	710.44	Joback Method
dvisc	0.0000349	Paxs	787.74	Joback Method
dvisc	0.0000228	Paxs	865.05	Joback Method
dvisc	0.0000160	Paxs	942.36	Joback Method
dvisc	0.0000118	Paxs	1019.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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