Adipic acid, hexyl tetradec-11-enyl ester

Inchi: InChI=1S/C26H48O4/c1-3-5-7-9-10-11-12-13-14-15-16-20-24-30-26(28)22-18-17-21-25(
InchiKey: PXWZUDVLYXZYHM-FNORWQNLSA-N
Formula: C26H48O4
SMILES: CCC=CCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-219.58	kJ/mol	Joback Method
hf	-952.35	kJ/mol	Joback Method
hfus	68.87	kJ/mol	Joback Method
hvap	91.74	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.691		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	784.63	kPa	Joback Method
rinpol	2925.00		NIST Webbook
tb	951.02	K	Joback Method
tc	1169.32	K	Joback Method
tf	522.02	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.56	J/mol×K	951.02	Joback Method
cpg	1338.32	J/mol×K	987.40	Joback Method
cpg	1357.57	J/mol×K	1023.79	Joback Method
cpg	1375.37	J/mol×K	1060.17	Joback Method
cpg	1391.79	J/mol×K	1096.55	Joback Method
cpg	1406.89	J/mol×K	1132.93	Joback Method
cpg	1420.74	J/mol×K	1169.32	Joback Method
dvisc	0.0003802	Pa×s	522.02	Joback Method
dvisc	0.0001707	Pa×s	593.52	Joback Method

dvisc	0.0000910	Pa×s	665.02	Joback Method
dvisc	0.0000548	Pa×s	736.52	Joback Method
dvisc	0.0000361	Pa×s	808.02	Joback Method
dvisc	0.0000255	Pa×s	879.52	Joback Method
dvisc	0.0000189	Pa×s	951.02	Joback Method

Sources

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=U353787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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