

Adipic acid, tetradecyl trans-hex-3-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(27)
InchiKey: QIABJKGMDGVFEW-SOFGYWHQSA-N
Formula: C26H48O4
SMILES: CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCC
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
mvol	387.780	ml/mol	McGowan Method
pc	784.63	kPa	Joback Method
rinpol	2925.00		NIST Webbook
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.56	J/molxK	951.02	Joback Method
cpg	1338.32	J/molxK	987.40	Joback Method
cpg	1357.57	J/molxK	1023.79	Joback Method
cpg	1375.37	J/molxK	1060.17	Joback Method
cpg	1391.79	J/molxK	1096.55	Joback Method
cpg	1406.89	J/molxK	1132.93	Joback Method
cpg	1420.74	J/molxK	1169.32	Joback Method
dvisc	0.0003802	Paxs	522.02	Joback Method

dvisc	0.0001707	Paxs	593.52	Joback Method
dvisc	0.0000910	Paxs	665.02	Joback Method
dvisc	0.0000548	Paxs	736.52	Joback Method
dvisc	0.0000361	Paxs	808.02	Joback Method
dvisc	0.0000255	Paxs	879.52	Joback Method
dvisc	0.0000189	Paxs	951.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354018&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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