

Adipic acid, pentadecyl pent-4-enyl ester

Inchi:	InChI=1S/C26H48O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-20-24-30-26(28)22-18-17-21-2
InchiKey:	PFVMOVOYSKLVQJ-UHFFFAOYSA-N
Formula:	C26H48O4
SMILES:	C=CCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	424.66

Physical Properties

Property code	Value	Unit	Source
gf	-211.96	kJ/mol	Joback Method
hf	-944.14	kJ/mol	Joback Method
hfus	67.39	kJ/mol	Joback Method
hvap	91.11	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.691		Crippen Method
mvol	387.780	ml/mol	McGowan Method
pc	780.25	kPa	Joback Method
rinpol	2916.00		NIST Webbook
tb	943.54	K	Joback Method
tc	1160.67	K	Joback Method
tf	525.34	K	Joback Method
vc	1.520	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.55	J/molxK	943.54	Joback Method
cpg	1336.29	J/molxK	979.73	Joback Method
cpg	1355.46	J/molxK	1015.92	Joback Method
cpg	1373.10	J/molxK	1052.11	Joback Method
cpg	1389.28	J/molxK	1088.30	Joback Method
cpg	1404.04	J/molxK	1124.48	Joback Method
cpg	1417.43	J/molxK	1160.67	Joback Method
dvisc	0.0004211	Paxs	525.34	Joback Method
dvisc	0.0001960	Paxs	595.04	Joback Method

dvisc	0.0001071	Paxs	664.74	Joback Method
dvisc	0.0000656	Paxs	734.44	Joback Method
dvisc	0.0000438	Paxs	804.14	Joback Method
dvisc	0.0000312	Paxs	873.84	Joback Method
dvisc	0.0000233	Paxs	943.54	Joback Method

Sources

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=U353804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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