

Adipic acid, pentadecyl trans-hex-3-enyl 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-SOFGYWHQSA-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
mvol	401.870	ml/mol	McGowan Method
pc	744.07	kPa	Joback Method
rinpol	3027.00		NIST Webbook
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tb	973.90	K	Joback Method
tc	1201.27	K	Joback Method
tf	533.29	K	Joback Method
vc	1.575	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001486	Paxs	606.72	Joback Method
dvisc	0.0000788	Paxs	680.16	Joback Method
dvisc	0.0000473	Paxs	753.60	Joback Method
dvisc	0.0000310	Paxs	827.03	Joback Method
dvisc	0.0000218	Paxs	900.46	Joback Method
dvisc	0.0000162	Paxs	973.90	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=U354019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	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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