

Adipic acid, hexadecyl pent-4-enyl ester

Inchi: InChI=1S/C27H50O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-21-25-31-27(29)23-19-18-2
InchiKey: ZPNLKORNZKTOPA-UHFFFAOYSA-N
Formula: C27H50O4
SMILES: C=CCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-203.54	kJ/mol	Joback Method
hf	-964.78	kJ/mol	Joback Method
hfus	69.98	kJ/mol	Joback Method
hvap	93.34	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.081		Crippen Method
mvol	401.870	ml/mol	McGowan Method
pc	740.03	kPa	Joback Method
rinpol	3028.00		NIST Webbook
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tb	966.42	K	Joback Method
tc	1192.80	K	Joback Method
tf	536.61	K	Joback Method
vc	1.577	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.69	J/molxK	966.42	Joback Method
cpg	1401.08	J/molxK	1004.15	Joback Method
cpg	1420.75	J/molxK	1041.88	Joback Method
cpg	1438.75	J/molxK	1079.61	Joback Method
cpg	1455.15	J/molxK	1117.34	Joback Method
cpg	1470.03	J/molxK	1155.07	Joback Method
cpg	1483.43	J/molxK	1192.80	Joback Method
dvisc	0.0003705	Paxs	536.61	Joback Method

dvisc	0.0001709	Paxs	608.25	Joback Method
dvisc	0.0000928	Paxs	679.88	Joback Method
dvisc	0.0000566	Paxs	751.52	Joback Method
dvisc	0.0000377	Paxs	823.15	Joback Method
dvisc	0.0000267	Paxs	894.79	Joback Method
dvisc	0.0000200	Paxs	966.42	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=U353805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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