

Adipic acid, cis-hex-3-enyl pentyl ester

Inchi:	InChI=1S/C17H30O4/c1-3-5-7-11-15-21-17(19)13-9-8-12-16(18)20-14-10-6-4-2/h5,7H,3-
InchiKey:	BDCSMFNERRYJJP-ALCCZGGFSA-N
Formula:	C17H30O4
SMILES:	CCC=CCCOC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	-295.36	kJ/mol	Joback Method
hf	-766.59	kJ/mol	Joback Method
hfus	45.56	kJ/mol	Joback Method
hvap	71.71	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.180		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1365.67	kPa	Joback Method
rinsol	2049.00		NIST Webbook
tb	745.10	K	Joback Method
tc	926.18	K	Joback Method
tf	420.59	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.28	J/molxK	745.10	Joback Method
cpg	841.29	J/molxK	896.00	Joback Method
cpg	828.12	J/molxK	865.82	Joback Method
cpg	814.15	J/molxK	835.64	Joback Method
cpg	799.37	J/molxK	805.46	Joback Method
cpg	783.75	J/molxK	775.28	Joback Method
cpg	853.69	J/molxK	926.18	Joback Method
dvisc	0.0000702	Paxs	745.10	Joback Method
dvisc	0.0000924	Paxs	691.01	Joback Method

dvisc	0.0001276	Paxs	636.93	Joback Method
dvisc	0.0001870	Paxs	582.84	Joback Method
dvisc	0.0002963	Paxs	528.76	Joback Method
dvisc	0.0005216	Paxs	474.67	Joback Method
dvisc	0.0010619	Paxs	420.59	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=U353973&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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