

Adipic acid, hexyl 3-methylbutyl ester

Inchi:	InChI=1S/C17H32O4/c1-4-5-6-9-13-20-16(18)10-7-8-11-17(19)21-14-12-15(2)3/h15H,4-
InchiKey:	PKUSJQIUSYROMX-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCCCOC(=O)CCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-378.02	kJ/mol	Joback Method
hf	-889.09	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	71.36	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.260		Crippen Method
mvol	265.270	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook
tb	740.50	K	Joback Method
tc	919.30	K	Joback Method
tf	410.67	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.52	J/molxK	740.50	Joback Method
cpg	808.68	J/molxK	770.30	Joback Method
cpg	824.95	J/molxK	800.10	Joback Method
cpg	840.35	J/molxK	829.90	Joback Method
cpg	854.88	J/molxK	859.70	Joback Method
cpg	868.56	J/molxK	889.50	Joback Method
cpg	881.39	J/molxK	919.30	Joback Method
dvisc	0.0013763	Paxs	410.67	Joback Method

dvisc	0.0006360	Paxs	465.64	Joback Method
dvisc	0.0003459	Paxs	520.61	Joback Method
dvisc	0.0002113	Paxs	575.59	Joback Method
dvisc	0.0001407	Paxs	630.56	Joback Method
dvisc	0.0001000	Paxs	685.53	Joback Method
dvisc	0.0000748	Paxs	740.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348968&Units=SI

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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