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,4-1
InchiKey: PKUSJQIUSYROMX-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CCCCCCOC(=O)CCCCC(=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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0006360	Pa×s	465.64	Joback Method
dvisc	0.0003459	Pa×s	520.61	Joback Method
dvisc	0.0002113	Pa×s	575.59	Joback Method
dvisc	0.0001407	Pa×s	630.56	Joback Method
dvisc	0.0001000	Pa×s	685.53	Joback Method
dvisc	0.0000748	Pa×s	740.50	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=U348968&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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