Adipic acid, 4-heptyl isobutyl ester

Inchi: InChI=1S/C17H32O4/c1-5-9-15(10-6-2)21-17(19)12-8-7-11-16(18)20-13-14(3)4/h14-15H
InchiKey: OBNUMOKKNVOHIG-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CCCC(CCC)OC(=O)CCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-380.46	kJ/mol	Joback Method
hf	-894.37	kJ/mol	Joback Method
hfus	38.31	kJ/mol	Joback Method
hvap	70.97	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.258		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
tb	740.06	K	Joback Method
tc	920.59	K	Joback Method
tf	395.67	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.00	J/mol×K	740.06	Joback Method
cpg	809.35	J/mol×K	770.15	Joback Method
cpg	825.78	J/mol×K	800.24	Joback Method
cpg	841.31	J/mol×K	830.32	Joback Method
cpg	855.95	J/mol×K	860.41	Joback Method
cpg	869.70	J/mol×K	890.50	Joback Method
cpg	882.59	J/mol×K	920.59	Joback Method
dvisc	0.0016971	Pa×s	395.67	Joback Method

dvisc	0.0007096	Pa×s	453.07	Joback Method
dvisc	0.0003610	Pa×s	510.47	Joback Method
dvisc	0.0002105	Pa×s	567.87	Joback Method
dvisc	0.0001355	Pa×s	625.26	Joback Method
dvisc	0.0000940	Pa×s	682.66	Joback Method
dvisc	0.0000690	Pa×s	740.06	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=U349736&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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