Adipic acid, isohexyl pent-4-enyl ester

Inchi: InChI=1S/C17H30O4/c1-4-5-8-13-20-16(18)11-6-7-12-17(19)21-14-9-10-15(2)3/h4,15H,1
InchiKey: DQGXHUOVOKREPW-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: C=CCCCOC(=O)CCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-290.18	kJ/mol	Joback Method
hf	-763.66	kJ/mol	Joback Method
hfus	40.56	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.036		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	737.18	K	Joback Method
tc	917.39	K	Joback Method
tf	408.91	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.33	J/mol×K	737.18	Joback Method
cpg	840.98	J/mol×K	887.36	Joback Method
cpg	827.74	J/mol×K	857.32	Joback Method
cpg	813.66	J/mol×K	827.29	Joback Method
cpg	798.75	J/mol×K	797.25	Joback Method
cpg	782.97	J/mol×K	767.22	Joback Method
cpg	853.40	J/mol×K	917.39	Joback Method
dvisc	0.0000793	Pa×s	737.18	Joback Method

dvisc	0.0001054	Pa×s	682.47	Joback Method
dvisc	0.0001473	Pa×s	627.76	Joback Method
dvisc	0.0002194	Pa×s	573.04	Joback Method
dvisc	0.0003555	Pa×s	518.33	Joback Method
dvisc	0.0006455	Pa×s	463.62	Joback Method
dvisc	0.0013750	Pa×s	408.91	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=U353794&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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