Adipic acid, pentyl trans-hex-3-enyl 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-FNORWQNLSA-N
Formula: C17H30O4
SMILES: CCC=CCCOC(=O)CCCCC(=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
rinpol	2040.00		NIST Webbook
tb	745.10	K	Joback Method
tc	926.18	K	Joback Method
tf	420.59	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001276	Pa×s	636.93	Joback Method
dvisc	0.0001870	Pa×s	582.84	Joback Method
dvisc	0.0002963	Pa×s	528.76	Joback Method
dvisc	0.0005216	Pa×s	474.67	Joback Method
dvisc	0.0010619	Pa×s	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=U354009&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