Pimelic acid, heptyl propyl ester

Inchi: InChI=1S/C17H32O4/c1-3-5-6-7-11-15-21-17(19)13-10-8-9-12-16(18)20-14-4-2/h3-15H2
InchiKey: XBNLFKRHABGHBI-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CCCCCCCOC(=O)CCCCCC(=O)OCCC
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-375.58	kJ/mol	Joback Method
hf	-883.81	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.404		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	1605.00		NIST Webbook
rinpol	1605.00		NIST Webbook
tb	740.94	K	Joback Method
tc	918.14	K	Joback Method
tf	425.67	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.03	J/mol×K	740.94	Joback Method
cpg	808.03	J/mol×K	770.47	Joback Method
cpg	824.15	J/mol×K	800.01	Joback Method
cpg	839.43	J/mol×K	829.54	Joback Method
cpg	853.86	J/mol×K	859.07	Joback Method
cpg	867.46	J/mol×K	888.60	Joback Method
cpg	880.23	J/mol×K	918.14	Joback Method
dvisc	0.0011435	Pa×s	425.67	Joback Method

dvisc	0.0005773	Pa×s	478.21	Joback Method
dvisc	0.0003337	Pa×s	530.76	Joback Method
dvisc	0.0002129	Pa×s	583.31	Joback Method
dvisc	0.0001463	Pa×s	635.85	Joback Method
dvisc	0.0001065	Pa×s	688.39	Joback Method
dvisc	0.0000811	Pa×s	740.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406508&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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