Pimelic acid, 2-methylpropyl pentyl ester

Inchi: InChI=1S/C16H30O4/c1-4-5-9-12-19-15(17)10-7-6-8-11-16(18)20-13-14(2)3/h14H,4-13H
InchiKey: UMXFZAUOMWOOTL-UHFFFAOYSA-N
Formula: C16H30O4
SMILES: CCCCCOC(=O)CCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-386.44	kJ/mol	Joback Method
hf	-868.45	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.870		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	717.62	K	Joback Method
tc	895.76	K	Joback Method
tf	399.40	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.08	J/mol×K	717.62	Joback Method
cpg	750.85	J/mol×K	747.31	Joback Method
cpg	766.77	J/mol×K	777.00	Joback Method
cpg	781.86	J/mol×K	806.69	Joback Method
cpg	796.13	J/mol×K	836.38	Joback Method
cpg	809.59	J/mol×K	866.07	Joback Method
cpg	822.23	J/mol×K	895.76	Joback Method
dvisc	0.0015210	Pa×s	399.40	Joback Method

dvisc	0.0007109	Pa×s	452.44	Joback Method
dvisc	0.0003898	Pa×s	505.47	Joback Method
dvisc	0.0002395	Pa×s	558.51	Joback Method
dvisc	0.0001602	Pa×s	611.55	Joback Method
dvisc	0.0001142	Pa×s	664.58	Joback Method
dvisc	0.0000856	Pa×s	717.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393852&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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