Pimelic acid, ethyl hexyl ester

Inchi: InChI=1S/C15H28O4/c1-3-5-6-10-13-19-15(17)12-9-7-8-11-14(16)18-4-2/h3-13H2,1-2H3
InchiKey: UNVQGXRYENKZPR-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CCCCCCOC(=O)CCCCCC(=O)OCC
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-392.42	kJ/mol	Joback Method
hf	-842.53	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.623		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
tb	695.18	K	Joback Method
tc	871.05	K	Joback Method
tf	403.13	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.29	J/mol×K	695.18	Joback Method
cpg	693.41	J/mol×K	724.49	Joback Method
cpg	708.76	J/mol×K	753.80	Joback Method
cpg	723.36	J/mol×K	783.12	Joback Method
cpg	737.19	J/mol×K	812.43	Joback Method
cpg	750.28	J/mol×K	841.74	Joback Method
cpg	762.62	J/mol×K	871.05	Joback Method
dvisc	0.0013699	Pa×s	403.13	Joback Method

dvisc	0.0007100	Pa×s	451.81	Joback Method
dvisc	0.0004181	Pa×s	500.48	Joback Method
dvisc	0.0002705	Pa×s	549.15	Joback Method
dvisc	0.0001878	Pa×s	597.83	Joback Method
dvisc	0.0001378	Pa×s	646.50	Joback Method
dvisc	0.0001056	Pa×s	695.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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