Pimelic acid, ethyl pentyl ester

Inchi: InChI=1S/C14H26O4/c1-3-5-9-12-18-14(16)11-8-6-7-10-13(15)17-4-2/h3-12H2,1-2H3
InchiKey: DVSYQMUZHLOEMY-UHFFFAOYSA-N
Formula: C14H26O4
SMILES: CCCCCOC(=O)CCCCCC(=O)OCC
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-400.84	kJ/mol	Joback Method
hf	-821.89	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	65.07	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.233		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1781.00		NIST Webbook
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tb	672.30	K	Joback Method
tc	848.26	K	Joback Method
tf	391.86	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.19	J/mol×K	672.30	Joback Method
cpg	637.83	J/mol×K	701.63	Joback Method
cpg	652.75	J/mol×K	730.95	Joback Method
cpg	666.95	J/mol×K	760.28	Joback Method
cpg	680.44	J/mol×K	789.61	Joback Method
cpg	693.22	J/mol×K	818.93	Joback Method
cpg	705.29	J/mol×K	848.26	Joback Method
dvisc	0.0014859	Pa×s	391.86	Joback Method

dvisc	0.0007810	Pa×s	438.60	Joback Method
dvisc	0.0004646	Pa×s	485.34	Joback Method
dvisc	0.0003028	Pa×s	532.08	Joback Method
dvisc	0.0002115	Pa×s	578.82	Joback Method
dvisc	0.0001558	Pa×s	625.56	Joback Method
dvisc	0.0001198	Pa×s	672.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393806&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