Pimelic acid, dodecyl ethyl ester

Inchi: InChI=1S/C21H40O4/c1-3-5-6-7-8-9-10-11-12-16-19-25-21(23)18-15-13-14-17-20(22)24
InchiKey: QBFDBIXZAZYCCS-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=O)OCC
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-341.90	kJ/mol	Joback Method
hf	-966.37	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	80.65	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.964		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1012.95	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	832.46	K	Joback Method
tc	1019.85	K	Joback Method
tf	470.75	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.26	J/mol×K	832.46	Joback Method
cpg	1048.96	J/mol×K	863.69	Joback Method
cpg	1066.54	J/mol×K	894.92	Joback Method
cpg	1083.03	J/mol×K	926.15	Joback Method
cpg	1098.44	J/mol×K	957.39	Joback Method
cpg	1112.80	J/mol×K	988.62	Joback Method
cpg	1126.13	J/mol×K	1019.85	Joback Method
dvisc	0.0007511	Pa×s	470.75	Joback Method

dvisc	0.0003622	Pa×s	531.03	Joback Method
dvisc	0.0002027	Pa×s	591.32	Joback Method
dvisc	0.0001263	Pa×s	651.61	Joback Method
dvisc	0.0000852	Pa×s	711.89	Joback Method
dvisc	0.0000612	Pa×s	772.17	Joback Method
dvisc	0.0000461	Pa×s	832.46	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=U406525&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