Pimelic acid, ethyl hexadecyl ester

Inchi: InChI=1S/C25H48O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-20-23-29-25(27)22-19-17-18
InchiKey: PNOMQOBLKBGGHE-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCC
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-308.22	kJ/mol	Joback Method
hf	-1048.93	kJ/mol	Joback Method
hfus	66.08	kJ/mol	Joback Method
hvap	89.56	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	7.524		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	804.33	kPa	Joback Method
rinpol	2867.00		NIST Webbook
rinpol	2867.00		NIST Webbook
tb	923.98	K	Joback Method
tc	1135.00	K	Joback Method
tf	515.83	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.17	J/mol×K	923.98	Joback Method
cpg	1301.94	J/mol×K	959.15	Joback Method
cpg	1321.17	J/mol×K	994.32	Joback Method
cpg	1338.92	J/mol×K	1029.49	Joback Method
cpg	1355.21	J/mol×K	1064.66	Joback Method
cpg	1370.09	J/mol×K	1099.83	Joback Method
cpg	1383.60	J/mol×K	1135.00	Joback Method
dvisc	0.0004642	Pa×s	515.83	Joback Method

dvisc	0.0002153	Pa×s	583.86	Joback Method
dvisc	0.0001173	Pa×s	651.88	Joback Method
dvisc	0.0000716	Pa×s	719.90	Joback Method
dvisc	0.0000476	Pa×s	787.93	Joback Method
dvisc	0.0000338	Pa×s	855.95	Joback Method
dvisc	0.0000252	Pa×s	923.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406547&Units=SI

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