Pimelic acid, 4-octyl tetradecyl ester

Inchi: InChI=1S/C29H56O4/c1-4-7-9-10-11-12-13-14-15-16-17-21-26-32-28(30)24-19-18-20-25
InchiKey: HRBZLRBWYWGOTM-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OC(CCC)CCCC
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-276.98	kJ/mol	Joback Method
hf	-1136.77	kJ/mol	Joback Method
hfus	72.92	kJ/mol	Joback Method
hvap	98.07	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	9.083		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	656.79	kPa	Joback Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	1015.06	K	Joback Method
tc	1265.21	K	Joback Method
tf	545.91	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.99	J/mol×K	1015.06	Joback Method
cpg	1563.19	J/mol×K	1056.75	Joback Method
cpg	1584.14	J/mol×K	1098.44	Joback Method
cpg	1602.93	J/mol×K	1140.13	Joback Method
cpg	1619.67	J/mol×K	1181.83	Joback Method
cpg	1634.42	J/mol×K	1223.52	Joback Method
cpg	1647.29	J/mol×K	1265.21	Joback Method
dvisc	0.0003091	Pa×s	545.91	Joback Method

dvisc	0.0001288	Pa×s	624.10	Joback Method
dvisc	0.0000652	Pa×s	702.29	Joback Method
dvisc	0.0000378	Pa×s	780.49	Joback Method
dvisc	0.0000242	Pa×s	858.68	Joback Method
dvisc	0.0000167	Pa×s	936.87	Joback Method
dvisc	0.0000122	Pa×s	1015.06	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=U406502&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