Pimelic acid, octyl tetradecyl ester

Inchi: InChI=1S/C29H56O4/c1-3-5-7-9-11-12-13-14-15-16-18-23-27-33-29(31)25-21-19-20-24-
InchiKey: FFQSYEZEFKTCJG-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-274.54	kJ/mol	Joback Method
hf	-1131.49	kJ/mol	Joback Method
hfus	76.44	kJ/mol	Joback Method
hvap	98.46	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	9.085		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	654.10	kPa	Joback Method
rinpol	3259.00		NIST Webbook
rinpol	3259.00		NIST Webbook
tb	1015.50	K	Joback Method
tc	1268.62	K	Joback Method
tf	560.91	K	Joback Method
vc	1.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.74	J/mol×K	1015.50	Joback Method
cpg	1563.27	J/mol×K	1057.69	Joback Method
cpg	1584.52	J/mol×K	1099.87	Joback Method
cpg	1603.59	J/mol×K	1142.06	Joback Method
cpg	1620.57	J/mol×K	1184.25	Joback Method
cpg	1635.54	J/mol×K	1226.44	Joback Method
cpg	1648.61	J/mol×K	1268.62	Joback Method
dvisc	0.0002741	Pa×s	560.91	Joback Method

dvisc	0.0001230	Pa×s	636.67	Joback Method
dvisc	0.0000654	Pa×s	712.44	Joback Method
dvisc	0.0000393	Pa×s	788.20	Joback Method
dvisc	0.0000258	Pa×s	863.97	Joback Method
dvisc	0.0000181	Pa×s	939.73	Joback Method
dvisc	0.0000134	Pa×s	1015.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393878&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

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

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