Pimelic acid, di(3,7-dimethyloctyl) ester

Inchi: InChI=1S/C27H52O4/c1-22(2)12-10-14-24(5)18-20-30-26(28)16-8-7-9-17-27(29)31-21-1
InchiKey: SNRQTBKMBPVSSZ-UHFFFAOYSA-N
Formula: C27H52O4
SMILES: CC(C)CCCC(C)CCOC(=O)CCCCCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-301.14	kJ/mol	Joback Method
hf	-1111.33	kJ/mol	Joback Method
hfus	57.17	kJ/mol	Joback Method
hvap	92.46	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.728		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	736.02	kPa	Joback Method
rinpol	2873.00		NIST Webbook
rinpol	2873.00		NIST Webbook
tb	967.98	K	Joback Method
tc	1190.47	K	Joback Method
tf	478.37	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1411.04	J/mol×K	967.98	Joback Method
cpg	1432.26	J/mol×K	1005.06	Joback Method
cpg	1451.69	J/mol×K	1042.14	Joback Method
cpg	1469.38	J/mol×K	1079.22	Joback Method
cpg	1485.37	J/mol×K	1116.30	Joback Method
cpg	1499.73	J/mol×K	1153.39	Joback Method
cpg	1512.51	J/mol×K	1190.47	Joback Method
dvisc	0.0006641	Pa×s	478.37	Joback Method

dvisc	0.0002125	Pa×s	559.97	Joback Method
dvisc	0.0000909	Pa×s	641.57	Joback Method
dvisc	0.0000471	Pa×s	723.17	Joback Method
dvisc	0.0000279	Pa×s	804.78	Joback Method
dvisc	0.0000182	Pa×s	886.38	Joback Method
dvisc	0.0000127	Pa×s	967.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393749&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