Pimelic acid, 3,7-dimethyloctyl tridecyl ester

Inchi: InChI=1S/C30H58O4/c1-5-6-7-8-9-10-11-12-13-14-18-25-33-29(31)22-16-15-17-23-30(3
InchiKey: SJWQEQKFVOZURZ-UHFFFAOYSA-N
Formula: C30H58O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	-271.00	kJ/mol	Joback Method
hf	-1162.69	kJ/mol	Joback Method
hfus	71.98	kJ/mol	Joback Method
hvap	99.91	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	9.187		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	628.14	kPa	Joback Method
rinpol	3253.00		NIST Webbook
rinpol	3253.00		NIST Webbook
tb	1037.50	K	Joback Method
tc	1297.92	K	Joback Method
tf	542.18	K	Joback Method
vc	1.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.60	J/mol×K	1037.50	Joback Method
cpg	1629.18	J/mol×K	1080.90	Joback Method
cpg	1650.31	J/mol×K	1124.31	Joback Method
cpg	1669.09	J/mol×K	1167.71	Joback Method
cpg	1685.63	J/mol×K	1211.11	Joback Method
cpg	1700.04	J/mol×K	1254.52	Joback Method
cpg	1712.42	J/mol×K	1297.92	Joback Method
dvisc	0.0003054	Pa×s	542.18	Joback Method

dvisc	0.0001167	Pa×s	624.73	Joback Method
dvisc	0.0000558	Pa×s	707.29	Joback Method
dvisc	0.0000312	Pa×s	789.84	Joback Method
dvisc	0.0000194	Pa×s	872.39	Joback Method
dvisc	0.0000131	Pa×s	954.95	Joback Method
dvisc	0.0000094	Pa×s	1037.50	Joback Method

Sources

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=U393746&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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