Pimelic acid, 3,7-dimethyloctyl pentadecyl ester

Inchi: InChI=1S/C32H62O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-20-27-35-31(33)24-18-17-19-2

InchiKey: UIVABDXXDHNJBQ-UHFFFAOYSA-N

Formula: C32H62O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCC(C)CCCC(C)C

Mol. weight [g/mol]: 510.83

Physical Properties

Property code	Value	Unit	Source
gf	-254.16	kJ/mol	Joback Method
hf	-1203.97	kJ/mol	Joback Method
hfus	77.16	kJ/mol	Joback Method
hvap	104.36	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	9.967		Crippen Method
mcvol	476.620	ml/mol	McGowan Method
pc	571.78	kPa	Joback Method
rinpol	3458.00		NIST Webbook
rinpol	3458.00		NIST Webbook
tb	1083.26	K	Joback Method
tc	1374.80	K	Joback Method
tf	564.72	K	Joback Method
vc	1.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.98	J/mol×K	1083.26	Joback Method
cpg	1833.76	J/mol×K	1326.21	Joback Method
cpg	1819.84	J/mol×K	1277.62	Joback Method
cpg	1803.37	J/mol×K	1229.03	Joback Method
cpg	1784.18	J/mol×K	1180.44	Joback Method
cpg	1762.10	J/mol×K	1131.85	Joback Method
cpg	1845.29	J/mol×K	1374.80	Joback Method
dvisc	0.0000068	Pa×s	1083.26	Joback Method

dvisc	0.0000095	Pa×s	996.84	Joback Method
dvisc	0.0000140	Pa×s	910.41	Joback Method
dvisc	0.0000226	Pa×s	823.99	Joback Method
dvisc	0.0000407	Pa×s	737.57	Joback Method
dvisc	0.0000857	Pa×s	651.14	Joback Method
dvisc	0.0002266	Pa×s	564.72	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=U393748&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