Pimelic acid, 3,7-dimethyloctyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C23H44O4/c1-18(2)11-10-12-20(5)15-16-26-22(24)13-8-7-9-14-23(25)27-21(6)17-19(3)4/h18-21H,7-17H2,1-6H3

InchiKey: TTZQTCFUANRIIV-UHFFFAOYSA-N

Formula: C23H44O4

SMILES: CC(C)CCCC(C)CCOC(=O)CCCCCC(=O)OC(C)CC(C)C

Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-334.82	kJ/mol	Joback Method
hf	-1028.77	kJ/mol	Joback Method
hfus	46.81	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.310		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	917.16	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	876.46	K	Joback Method
tc	1073.32	K	Joback Method
tf	433.29	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.28	J/mol×K	876.46	Joback Method
cpg	1175.85	J/mol×K	909.27	Joback Method
cpg	1194.08	J/mol×K	942.08	Joback Method
cpg	1211.02	J/mol×K	974.89	Joback Method
cpg	1226.67	J/mol×K	1007.70	Joback Method
cpg	1241.08	J/mol×K	1040.51	Joback Method
cpg	1254.27	J/mol×K	1073.32	Joback Method
dvisc	0.0012150	Pa×s	433.29	Joback Method

dvisc	0.0003922	Pa×s	507.15	Joback Method
dvisc	0.0001688	Pa×s	581.01	Joback Method
dvisc	0.0000878	Pa×s	654.88	Joback Method
dvisc	0.0000522	Pa×s	728.74	Joback Method
dvisc	0.0000341	Pa×s	802.60	Joback Method
dvisc	0.0000240	Pa×s	876.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393738&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