Pimelic acid, 4-methyl-2-pentyl 3-phenylpropyl ester

Inchi: InChI=1S/C22H34O4/c1-18(2)17-19(3)26-22(24)15-9-5-8-14-21(23)25-16-10-13-20-11-6

InchiKey: GXAGWHDYQDXRMW-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-225.95	kJ/mol	Joback Method
hf	-761.04	kJ/mol	Joback Method
hfus	45.30	kJ/mol	Joback Method
hvap	84.38	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.091		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
tb	881.14	K	Joback Method
tc	1085.73	K	Joback Method
tf	478.44	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.81	J/mol×K	881.14	Joback Method
cpg	1015.61	J/mol×K	915.24	Joback Method
cpg	1031.13	J/mol×K	949.34	Joback Method
cpg	1045.41	J/mol×K	983.44	Joback Method
cpg	1058.50	J/mol×K	1017.53	Joback Method
cpg	1070.42	J/mol×K	1051.63	Joback Method
cpg	1081.21	J/mol×K	1085.73	Joback Method
dvisc	0.0007415	Pa×s	478.44	Joback Method

dvisc	0.0003233	Pa×s	545.56	Joback Method
dvisc	0.0001691	Pa×s	612.67	Joback Method
dvisc	0.0001005	Pa×s	679.79	Joback Method
dvisc	0.0000656	Pa×s	746.91	Joback Method
dvisc	0.0000459	Pa×s	814.02	Joback Method
dvisc	0.0000340	Pa×s	881.14	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=U416511&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