Pimelic acid, 4-methyl-2-pentyl 2-methoxyphenyl ester

Inchi: InChI=1S/C20H30O5/c1-15(2)14-16(3)24-19(21)12-6-5-7-13-20(22)25-18-11-9-8-10-17(1

InchiKey: MTHYCHUQTBHKKZ-UHFFFAOYSA-N

Formula: C20H30O5

SMILES: COc1ccccc1OC(=O)CCCCCC(=O)OC(C)CC(C)C

Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-357.42	kJ/mol	Joback Method
hf	-863.45	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.529		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	862.78	K	Joback Method
tc	1067.37	K	Joback Method
tf	490.65	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.12	J/mol×K	862.78	Joback Method
cpg	923.97	J/mol×K	896.88	Joback Method
cpg	938.54	J/mol×K	930.98	Joback Method
cpg	951.85	J/mol×K	965.07	Joback Method
cpg	963.92	J/mol×K	999.17	Joback Method
cpg	974.74	J/mol×K	1033.27	Joback Method
cpg	984.34	J/mol×K	1067.37	Joback Method
dvisc	0.0005303	Pa×s	490.65	Joback Method

dvisc	0.0002604	Pa×s	552.67	Joback Method
dvisc	0.0001476	Pa×s	614.69	Joback Method
dvisc	0.0000928	Pa×s	676.72	Joback Method
dvisc	0.0000631	Pa×s	738.74	Joback Method
dvisc	0.0000455	Pa×s	800.76	Joback Method
dvisc	0.0000344	Pa×s	862.78	Joback Method

Sources

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=U416524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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