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

Inchi: InChI=1S/C21H32O5/c1-16(2)14-17(3)26-21(23)9-7-5-6-8-20(22)25-15-18-10-12-19(24-4

InchiKey: OIZCZXTYKJNMHK-UHFFFAOYSA-N

Formula: C21H32O5

SMILES: COc1ccc(COC(=O)CCCCCC(=O)OC(C)CC(C)C)cc1

Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-349.00	kJ/mol	Joback Method
hf	-884.09	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	85.22	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.667		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2706.00		NIST Webbook
rinpol	2706.00		NIST Webbook
tb	885.66	K	Joback Method
tc	1091.46	K	Joback Method
tf	501.92	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.72	J/mol×K	885.66	Joback Method
cpg	1034.38	J/mol×K	1057.16	Joback Method
cpg	1023.65	J/mol×K	1022.86	Joback Method
cpg	1011.63	J/mol×K	988.56	Joback Method
cpg	998.32	J/mol×K	954.26	Joback Method
cpg	983.68	J/mol×K	919.96	Joback Method
cpg	1043.83	J/mol×K	1091.46	Joback Method
dvisc	0.0000298	Pa×s	885.66	Joback Method

dvisc	0.0000394	Pa×s	821.70	Joback Method
dvisc	0.0000548	Pa×s	757.75	Joback Method
dvisc	0.0000809	Pa×s	693.79	Joback Method
dvisc	0.0001293	Pa×s	629.83	Joback Method
dvisc	0.0002299	Pa×s	565.88	Joback Method
dvisc	0.0004729	Pa×s	501.92	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=U416540&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