

# Pimelic acid, heptyl 4-methoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C22H34O5/c1-3-4-5-6-10-17-26-21(23)11-8-7-9-12-22(24)27-18-19-13-15-20(2)
<b>InchiKey:</b>	CFXGOWRRRVKFDH-UHFFFAOYSA-N
<b>Formula:</b>	C22H34O5
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCC(=O)OCc1ccc(OC)cc1
<b>Mol. weight [g/mol]:</b>	378.50

## Physical Properties

Property code	Value	Unit	Source
gf	-335.70	kJ/mol	Joback Method
hf	-894.17	kJ/mol	Joback Method
hfus	53.15	kJ/mol	Joback Method
hvap	88.23	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.202		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinsol	2915.00		NIST Webbook
tb	909.42	K	Joback Method
tc	1115.54	K	Joback Method
tf	543.19	K	Joback Method
vc	1.226	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.01	J/molxK	909.42	Joback Method
cpg	1043.01	J/molxK	943.77	Joback Method
cpg	1057.67	J/molxK	978.13	Joback Method
cpg	1070.99	J/molxK	1012.48	Joback Method
cpg	1082.99	J/molxK	1046.83	Joback Method
cpg	1093.70	J/molxK	1081.18	Joback Method
cpg	1103.12	J/molxK	1115.54	Joback Method
dvisc	0.0003352	Paxs	543.19	Joback Method
dvisc	0.0001841	Paxs	604.23	Joback Method

dvisc	0.0001129	Paxs	665.27	Joback Method
dvisc	0.0000751	Paxs	726.31	Joback Method
dvisc	0.0000532	Paxs	787.34	Joback Method
dvisc	0.0000397	Paxs	848.38	Joback Method
dvisc	0.0000307	Paxs	909.42	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416542&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416542&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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