

# Pimelic acid, hexyl 2-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C20H30O4/c1-3-4-5-11-16-23-19(21)14-7-6-8-15-20(22)24-18-13-10-9-12-17(
<b>InchiKey:</b>	YKULFIXUGWZGOV-UHFFFAOYSA-N
<b>Formula:</b>	C20H30O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCC(=O)Oc1ccccc1C
<b>Mol. weight [g/mol]:</b>	334.45

## Physical Properties

Property code	Value	Unit	Source
gf	-247.54	kJ/mol	Joback Method
hf	-720.67	kJ/mol	Joback Method
hfus	46.78	kJ/mol	Joback Method
hvap	81.36	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.974		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2755.00		NIST Webbook
rinpol	2755.00		NIST Webbook
tb	841.24	K	Joback Method
tc	1041.25	K	Joback Method
tf	498.42	K	Joback Method
vc	1.095	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.72	J/molxK	841.24	Joback Method
cpg	893.85	J/molxK	874.57	Joback Method
cpg	908.85	J/molxK	907.91	Joback Method
cpg	922.75	J/molxK	941.24	Joback Method
cpg	935.56	J/molxK	974.58	Joback Method
cpg	947.32	J/molxK	1007.91	Joback Method
cpg	958.03	J/molxK	1041.25	Joback Method
dvisc	0.0005930	Paxs	498.42	Joback Method

dvisc	0.0003251	Paxs	555.56	Joback Method
dvisc	0.0001994	Paxs	612.69	Joback Method
dvisc	0.0001329	Paxs	669.83	Joback Method
dvisc	0.0000945	Paxs	726.97	Joback Method
dvisc	0.0000705	Paxs	784.10	Joback Method
dvisc	0.0000548	Paxs	841.24	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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=U416488&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416488&amp;Units=SI</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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