

# Pimelic acid, decyl phenethyl ester

<b>Inchi:</b>	InChI=1S/C25H40O4/c1-2-3-4-5-6-7-8-15-21-28-24(26)18-13-10-14-19-25(27)29-22-20-2
<b>InchiKey:</b>	BAKQCOUZAZOLOA-UHFFFAOYSA-N
<b>Formula:</b>	C25H40O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCC(=O)OCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	404.58

## Physical Properties

Property code	Value	Unit	Source
gf	-195.81	kJ/mol	Joback Method
hf	-812.40	kJ/mol	Joback Method
hfus	60.12	kJ/mol	Joback Method
hvap	91.83	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.407		Crippen Method
mvol	354.230	ml/mol	McGowan Method
pc	979.62	kPa	Joback Method
rinpol	3072.00		NIST Webbook
rinpol	3072.00		NIST Webbook
tb	950.66	K	Joback Method
tc	1163.88	K	Joback Method
tf	542.25	K	Joback Method
vc	1.375	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.85	J/molxK	950.66	Joback Method
cpg	1255.10	J/molxK	1128.34	Joback Method
cpg	1243.10	J/molxK	1092.80	Joback Method
cpg	1229.82	J/molxK	1057.27	Joback Method
cpg	1215.22	J/molxK	1021.73	Joback Method
cpg	1199.24	J/molxK	986.20	Joback Method
cpg	1265.88	J/molxK	1163.88	Joback Method
dvisc	0.0000259	Paxs	950.66	Joback Method

dvisc	0.0000343	Paxs	882.59	Joback Method
dvisc	0.0000475	Paxs	814.52	Joback Method
dvisc	0.0000697	Paxs	746.45	Joback Method
dvisc	0.0001106	Paxs	678.39	Joback Method
dvisc	0.0001945	Paxs	610.32	Joback Method
dvisc	0.0003943	Paxs	542.25	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416502&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416502&amp;Units=SI</a>
<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>

## 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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