

# Pimelic acid, isobutyl 1-naphthyl ester

<b>Inchi:</b>	InChI=1S/C21H26O4/c1-16(2)15-24-20(22)13-4-3-5-14-21(23)25-19-12-8-10-17-9-6-7-1
<b>InchiKey:</b>	UAGUSUZZSMVIAN-UHFFFAOYSA-N
<b>Formula:</b>	C21H26O4
<b>SMILES:</b>	CC(C)COC(=O)CCCCC(=O)Oc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	342.43

## Physical Properties

Property code	Value	Unit	Source
gf	-134.91	kJ/mol	Joback Method
hf	-555.52	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.895		Crippen Method
mvol	278.410	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	882.66	K	Joback Method
tc	1098.28	K	Joback Method
tf	527.39	K	Joback Method
vc	1.067	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.57	J/molxK	882.66	Joback Method
cpg	876.41	J/molxK	918.60	Joback Method
cpg	890.13	J/molxK	954.53	Joback Method
cpg	902.78	J/molxK	990.47	Joback Method
cpg	914.42	J/molxK	1026.41	Joback Method
cpg	925.10	J/molxK	1062.35	Joback Method
cpg	934.88	J/molxK	1098.28	Joback Method
dvisc	0.0007083	Paxs	527.39	Joback Method

dvisc	0.0004187	Paxs	586.60	Joback Method
dvisc	0.0002725	Paxs	645.81	Joback Method
dvisc	0.0001907	Paxs	705.03	Joback Method
dvisc	0.0001410	Paxs	764.24	Joback Method
dvisc	0.0001089	Paxs	823.45	Joback Method
dvisc	0.0000871	Paxs	882.66	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=U416718&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416718&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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