

# Pimelic acid, nonyl pentafluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C23H31F5O4/c1-2-3-4-5-6-7-11-14-31-17(29)12-9-8-10-13-18(30)32-15-16-19
<b>InchiKey:</b>	HFBQOEQUJOFGJR-UHFFFAOYSA-N
<b>Formula:</b>	C23H31F5O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	466.48

## Physical Properties

Property code	Value	Unit	Source
gf	-1234.85	kJ/mol	Joback Method
hf	-1809.02	kJ/mol	Joback Method
hfus	68.40	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	6.670		Crippen Method
mvol	334.900	ml/mol	McGowan Method
pc	916.61	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	926.15	K	Joback Method
tc	1136.96	K	Joback Method
tf	585.26	K	Joback Method
vc	1.353	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.84	J/mol×K	926.15	Joback Method
cpg	1106.71	J/mol×K	961.28	Joback Method
cpg	1121.19	J/mol×K	996.42	Joback Method
cpg	1134.29	J/mol×K	1031.55	Joback Method
cpg	1146.04	J/mol×K	1066.69	Joback Method
cpg	1156.46	J/mol×K	1101.82	Joback Method
cpg	1165.55	J/mol×K	1136.96	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416633&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416633&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>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>hvp:</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>rinp:</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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