

# Pimelic acid, hexyl 2-nitro-5-fluorophenyl ester

<b>Inchi:</b>	InChI=1S/C19H26FNO6/c1-2-3-4-8-13-26-18(22)9-6-5-7-10-19(23)27-17-14-15(20)11-12
<b>InchiKey:</b>	ZDRMGJSEIVYFOU-UHFFFAOYSA-N
<b>Formula:</b>	C19H26FNO6
<b>SMILES:</b>	CCCCCOC(=O)CCCCC(=O)Oc1cc(F)ccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	383.41

## Physical Properties

Property code	Value	Unit	Source
gf	-424.85	kJ/mol	Joback Method
hf	-918.37	kJ/mol	Joback Method
hfus	58.24	kJ/mol	Joback Method
hvap	95.57	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.713		Crippen Method
mvol	288.880	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	2740.00		NIST Webbook
rinpol	2740.00		NIST Webbook
tb	974.45	K	Joback Method
tc	1196.30	K	Joback Method
tf	643.87	K	Joback Method
vc	1.139	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.80	J/molxK	974.45	Joback Method
cpg	946.88	J/molxK	1011.43	Joback Method
cpg	957.67	J/molxK	1048.40	Joback Method
cpg	967.19	J/molxK	1085.38	Joback Method
cpg	975.46	J/molxK	1122.35	Joback Method
cpg	982.51	J/molxK	1159.33	Joback Method
cpg	988.38	J/molxK	1196.30	Joback Method

# Sources

<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=U416477&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416477&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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>r in pol:</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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