

# Isophthalic acid, ethyl pentafluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C17H11F5O4/c1-2-25-16(23)8-4-3-5-9(6-8)17(24)26-7-10-11(18)13(20)15(22)
<b>InchiKey:</b>	HINCOPCIUMJKMZ-UHFFFAOYSA-N
<b>Formula:</b>	C17H11F5O4
<b>SMILES:</b>	CCOC(=O)c1cccc(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1
<b>Mol. weight [g/mol]:</b>	374.26

## Physical Properties

Property code	Value	Unit	Source
gf	-1182.59	kJ/mol	Joback Method
hf	-1460.12	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	76.19	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	3.916		Crippen Method
mcvol	226.600	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
tb	820.53	K	Joback Method
tc	1022.07	K	Joback Method
tf	556.58	K	Joback Method
vc	0.909	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.99	J/mol×K	820.53	Joback Method
cpg	654.85	J/mol×K	854.12	Joback Method
cpg	664.80	J/mol×K	887.71	Joback Method
cpg	673.85	J/mol×K	921.30	Joback Method
cpg	681.98	J/mol×K	954.89	Joback Method
cpg	689.20	J/mol×K	988.48	Joback Method
cpg	695.52	J/mol×K	1022.07	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U344502&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344502&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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