

# Phthalic acid, 3-fluorophenyl propyl ester

<b>Inchi:</b>	InChI=1S/C17H15FO4/c1-2-10-21-16(19)14-8-3-4-9-15(14)17(20)22-13-7-5-6-12(18)11-
<b>InchiKey:</b>	ZAIYZFMKSPJCDI-UHFFFAOYSA-N
<b>Formula:</b>	C17H15FO4
<b>SMILES:</b>	CCCOC(=O)c1ccccc1C(=O)Oc1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	302.30

## Physical Properties

Property code	Value	Unit	Source
gf	-364.83	kJ/mol	Joback Method
hf	-629.80	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	76.81	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.612		Crippen Method
mvol	219.520	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	803.53	K	Joback Method
tc	1027.80	K	Joback Method
tf	504.14	K	Joback Method
vc	0.838	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.17	J/mol×K	803.53	Joback Method
cpg	632.24	J/mol×K	840.91	Joback Method
cpg	644.17	J/mol×K	878.29	Joback Method
cpg	654.97	J/mol×K	915.66	Joback Method
cpg	664.68	J/mol×K	953.04	Joback Method
cpg	673.31	J/mol×K	990.42	Joback Method
cpg	680.88	J/mol×K	1027.80	Joback Method

# Sources

<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=U356498&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356498&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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