

# Phthalic acid, ethyl 3-fluorophenyl ester

<b>Inchi:</b>	InChI=1S/C16H13FO4/c1-2-20-15(18)13-8-3-4-9-14(13)16(19)21-12-7-5-6-11(17)10-12/H
<b>InchiKey:</b>	ZJWHDXWVRDYSTB-UHFFFAOYSA-N
<b>Formula:</b>	C16H13FO4
<b>SMILES:</b>	CCOC(=O)c1ccccc1C(=O)Oc1ccc(F)c1
<b>Mol. weight [g/mol]:</b>	288.27

## Physical Properties

Property code	Value	Unit	Source
gf	-373.25	kJ/mol	Joback Method
hf	-609.16	kJ/mol	Joback Method
hfus	33.15	kJ/mol	Joback Method
hvap	74.58	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.222		Crippen Method
mcvol	205.430	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	780.65	K	Joback Method
tc	1008.11	K	Joback Method
tf	492.87	K	Joback Method
vc	0.781	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.83	J/molxK	780.65	Joback Method
cpg	577.63	J/molxK	818.56	Joback Method
cpg	589.32	J/molxK	856.47	Joback Method
cpg	599.90	J/molxK	894.38	Joback Method
cpg	609.41	J/molxK	932.29	Joback Method
cpg	617.85	J/molxK	970.20	Joback Method
cpg	625.26	J/molxK	1008.11	Joback Method

# Sources

<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=U356499&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356499&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>

# 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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