

# Isophthalic acid, butyl 3-fluorophenyl ester

<b>Inchi:</b>	InChI=1S/C18H17FO4/c1-2-3-10-22-17(20)13-6-4-7-14(11-13)18(21)23-16-9-5-8-15(19)
<b>InchiKey:</b>	WTDMMQPLDOYDEQ-UHFFFAOYSA-N
<b>Formula:</b>	C18H17FO4
<b>SMILES:</b>	CCCCOC(=O)c1cccc(C(=O)Oc2cccc(F)c2)c1
<b>Mol. weight [g/mol]:</b>	316.32

## Physical Properties

Property code	Value	Unit	Source
gf	-356.41	kJ/mol	Joback Method
hf	-650.44	kJ/mol	Joback Method
hfus	38.33	kJ/mol	Joback Method
hvap	79.03	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.002		Crippen Method
mvol	233.610	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2425.00		NIST Webbook
rinpol	2425.00		NIST Webbook
tb	826.41	K	Joback Method
tc	1048.06	K	Joback Method
tf	515.41	K	Joback Method
vc	0.893	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.47	J/mol×K	826.41	Joback Method
cpg	687.76	J/mol×K	863.35	Joback Method
cpg	699.87	J/mol×K	900.29	Joback Method
cpg	710.85	J/mol×K	937.23	Joback Method
cpg	720.70	J/mol×K	974.18	Joback Method
cpg	729.47	J/mol×K	1011.12	Joback Method
cpg	737.16	J/mol×K	1048.06	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U344667&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344667&amp;Units=SI</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>hvap:</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>rinpola:</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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