

# Isophthalic acid, 2-fluorophenyl hexyl ester

<b>Inchi:</b>	InChI=1S/C20H21FO4/c1-2-3-4-7-13-24-19(22)15-9-8-10-16(14-15)20(23)25-18-12-6-5-
<b>InchiKey:</b>	DAXPTGGEMQUOCP-UHFFFAOYSA-N
<b>Formula:</b>	C20H21FO4
<b>SMILES:</b>	CCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2F)c1
<b>Mol. weight [g/mol]:</b>	344.38

## Physical Properties

Property code	Value	Unit	Source
gf	-339.57	kJ/mol	Joback Method
hf	-691.72	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	83.48	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.782		Crippen Method
mvol	261.790	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2645.00		NIST Webbook
rinpol	2645.00		NIST Webbook
tb	872.17	K	Joback Method
tc	1090.48	K	Joback Method
tf	537.95	K	Joback Method
vc	1.006	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.68	J/mol×K	872.17	Joback Method
cpg	801.27	J/mol×K	908.56	Joback Method
cpg	813.65	J/mol×K	944.94	Joback Method
cpg	824.84	J/mol×K	981.33	Joback Method
cpg	834.86	J/mol×K	1017.71	Joback Method
cpg	843.76	J/mol×K	1054.10	Joback Method
cpg	851.56	J/mol×K	1090.48	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=U344655&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344655&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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