

# Isophthalic acid, decyl 2-fluorophenyl ester

**Inchi:** InChI=1S/C24H29FO4/c1-2-3-4-5-6-7-8-11-17-28-23(26)19-13-12-14-20(18-19)24(27)29  
**InchiKey:** SIYZCENRSALRGZ-UHFFFAOYSA-N  
**Formula:** C24H29FO4  
**SMILES:** CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2F)c1  
**Mol. weight [g/mol]:** 400.48

## Physical Properties

Property code	Value	Unit	Source
gf	-305.89	kJ/mol	Joback Method
hf	-774.28	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	92.39	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	6.342		Crippen Method
mvol	318.150	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	3076.00		NIST Webbook
rinpol	3076.00		NIST Webbook
tb	963.69	K	Joback Method
tc	1184.18	K	Joback Method
tf	583.03	K	Joback Method
vc	1.230	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1022.64	J/molxK	963.69	Joback Method
cpg	1036.65	J/molxK	1000.44	Joback Method
cpg	1049.29	J/molxK	1037.19	Joback Method
cpg	1060.60	J/molxK	1073.94	Joback Method
cpg	1070.64	J/molxK	1110.68	Joback Method
cpg	1079.45	J/molxK	1147.43	Joback Method
cpg	1087.07	J/molxK	1184.18	Joback Method

# Sources

<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=U344659&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344659&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>

# 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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