

# Phthalic acid, 3-fluorophenyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C27H35FO4/c1-2-3-4-5-6-7-8-9-10-11-14-20-31-26(29)24-18-12-13-19-25(24)
<b>InchiKey:</b>	FHMZBEFBKJRKX-UHFFFAOYSA-N
<b>Formula:</b>	C27H35FO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	442.56

## Physical Properties

Property code	Value	Unit	Source
gf	-280.63	kJ/mol	Joback Method
hf	-836.20	kJ/mol	Joback Method
hfus	61.64	kJ/mol	Joback Method
hvap	99.07	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	7.513		Crippen Method
mvol	360.420	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	3148.00		NIST Webbook
rinpol	3148.00		NIST Webbook
tb	1032.33	K	Joback Method
tc	1263.87	K	Joback Method
tf	616.84	K	Joback Method
vc	1.397	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.53	J/molxK	1032.33	Joback Method
cpg	1218.88	J/molxK	1070.92	Joback Method
cpg	1231.68	J/molxK	1109.51	Joback Method
cpg	1242.99	J/molxK	1148.10	Joback Method
cpg	1252.87	J/molxK	1186.69	Joback Method
cpg	1261.39	J/molxK	1225.28	Joback Method
cpg	1268.61	J/molxK	1263.87	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356667&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356667&amp;Units=SI</a>
<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>

# 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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