

# Phthalic acid, 3-fluorophenyl tetradecyl ester

**Inchi:** InChI=1S/C28H37FO4/c1-2-3-4-5-6-7-8-9-10-11-12-15-21-32-27(30)25-19-13-14-20-26(27)  
**InchiKey:** KDLIGHUZRHHOAG-UHFFFAOYSA-N  
**Formula:** C28H37FO4  
**SMILES:** CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccc(F)c1  
**Mol. weight [g/mol]:** 456.59

## Physical Properties

Property code	Value	Unit	Source
gf	-272.21	kJ/mol	Joback Method
hf	-856.84	kJ/mol	Joback Method
hfus	64.23	kJ/mol	Joback Method
hvap	101.29	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	7.903		Crippen Method
mvol	374.510	ml/mol	McGowan Method
pc	960.29	kPa	Joback Method
rinpol	3253.00		NIST Webbook
rinpol	3253.00		NIST Webbook
tb	1055.21	K	Joback Method
tc	1292.56	K	Joback Method
tf	628.11	K	Joback Method
vc	1.454	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1265.98	J/molxK	1055.21	Joback Method
cpg	1280.48	J/molxK	1094.77	Joback Method
cpg	1293.34	J/molxK	1134.33	Joback Method
cpg	1304.64	J/molxK	1173.88	Joback Method
cpg	1314.44	J/molxK	1213.44	Joback Method
cpg	1322.83	J/molxK	1253.00	Joback Method
cpg	1329.88	J/molxK	1292.56	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.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>
<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=U356666&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356666&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>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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