

# Terephthalic acid, 2-fluorobenzyl octyl ester

**Inchi:** InChI=1S/C23H27FO4/c1-2-3-4-5-6-9-16-27-22(25)18-12-14-19(15-13-18)23(26)28-17-2  
**InchiKey:** FVCUBAIGIHGZSZ-UHFFFAOYSA-N  
**Formula:** C23H27FO4  
**SMILES:** CCCCCCOC(=O)c1ccc(C(=O)OCc2ccccc2F)cc1  
**Mol. weight [g/mol]:** 386.46

## Physical Properties

Property code	Value	Unit	Source
gf	-314.31	kJ/mol	Joback Method
hf	-753.64	kJ/mol	Joback Method
hfus	51.28	kJ/mol	Joback Method
hvap	90.16	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	5.700		Crippen Method
mcvol	304.060	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinsol	3318.00		NIST Webbook
rinsol	3318.00		NIST Webbook
tb	940.81	K	Joback Method
tc	1159.53	K	Joback Method
tf	571.76	K	Joback Method
vc	1.173	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.99	J/molxK	940.81	Joback Method
cpg	976.89	J/molxK	977.26	Joback Method
cpg	989.48	J/molxK	1013.72	Joback Method
cpg	1000.79	J/molxK	1050.17	Joback Method
cpg	1010.85	J/molxK	1086.62	Joback Method
cpg	1019.72	J/molxK	1123.07	Joback Method
cpg	1027.43	J/molxK	1159.53	Joback Method

# Sources

<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=U383016&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383016&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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