

# Phthalic acid, 3-fluorobenzyl heptyl ester

<b>Inchi:</b>	InChI=1S/C22H25FO4/c1-2-3-4-5-8-14-26-21(24)19-12-6-7-13-20(19)22(25)27-16-17-10
<b>InchiKey:</b>	YWLNDBHUGVPYLH-UHFFFAOYSA-N
<b>Formula:</b>	C22H25FO4
<b>SMILES:</b>	CCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	372.43

## Physical Properties

Property code	Value	Unit	Source
gf	-322.73	kJ/mol	Joback Method
hf	-733.00	kJ/mol	Joback Method
hfus	48.69	kJ/mol	Joback Method
hvap	87.94	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	5.310		Crippen Method
mvol	289.970	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	2653.00		NIST Webbook
rinpol	2653.00		NIST Webbook
tb	917.93	K	Joback Method
tc	1135.73	K	Joback Method
tf	560.49	K	Joback Method
vc	1.117	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.90	J/molxK	917.93	Joback Method
cpg	917.71	J/molxK	954.23	Joback Method
cpg	930.24	J/molxK	990.53	Joback Method
cpg	941.53	J/molxK	1026.83	Joback Method
cpg	951.60	J/molxK	1063.13	Joback Method
cpg	960.51	J/molxK	1099.43	Joback Method
cpg	968.28	J/molxK	1135.73	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=U377892&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377892&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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