

# Terephthalic acid, butyl 2-fluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C19H19FO4/c1-2-3-12-23-18(21)14-8-10-15(11-9-14)19(22)24-13-16-6-4-5-7-
<b>InchiKey:</b>	VNGVCGJKNPSPSD-UHFFFAOYSA-N
<b>Formula:</b>	C19H19FO4
<b>SMILES:</b>	CCCCOC(=O)c1ccc(C(=O)OCc2ccccc2F)cc1
<b>Mol. weight [g/mol]:</b>	330.35

## Physical Properties

Property code	Value	Unit	Source
gf	-347.99	kJ/mol	Joback Method
hf	-671.08	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	81.26	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.140		Crippen Method
mcvol	247.700	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpola	2898.00		NIST Webbook
rinpola	2898.00		NIST Webbook
tb	849.29	K	Joback Method
tc	1068.94	K	Joback Method
tf	526.68	K	Joback Method
vc	0.950	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.66	J/mol×K	849.29	Joback Method
cpg	744.12	J/mol×K	885.90	Joback Method
cpg	756.39	J/mol×K	922.51	Joback Method
cpg	767.48	J/mol×K	959.12	Joback Method
cpg	777.44	J/mol×K	995.72	Joback Method
cpg	786.29	J/mol×K	1032.33	Joback Method
cpg	794.06	J/mol×K	1068.94	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U383012&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383012&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>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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