

# Phthalic acid, butyl 2,2,2-trifluoro-1-phenylethyl ester

<b>Inchi:</b>	InChI=1S/C20H19F3O4/c1-2-3-13-26-18(24)15-11-7-8-12-16(15)19(25)27-17(20(21,22)23)
<b>InchiKey:</b>	KPPRJXBUIOUORGV-UHFFFAOYSA-N
<b>Formula:</b>	C20H19F3O4
<b>SMILES:</b>	CCCCOC(=O)c1ccccc1C(=O)OC(c1ccccc1)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	380.36

## Physical Properties

Property code	Value	Unit	Source
gf	-719.16	kJ/mol	Joback Method
hf	-1086.50	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	79.50	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.104		Crippen Method
mvol	265.330	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2190.00		NIST Webbook
tb	862.06	K	Joback Method
tc	1077.35	K	Joback Method
tf	514.03	K	Joback Method
vc	1.024	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.20	J/mol×K	862.06	Joback Method
cpg	818.27	J/mol×K	897.94	Joback Method
cpg	830.18	J/mol×K	933.82	Joback Method
cpg	840.99	J/mol×K	969.71	Joback Method
cpg	850.77	J/mol×K	1005.59	Joback Method
cpg	859.56	J/mol×K	1041.47	Joback Method
cpg	867.44	J/mol×K	1077.35	Joback Method

# Sources

<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=U377702&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377702&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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