

# Terephthalic acid, pentyl 3,4,5-trifluorobenzyl ester

Inchi:	InChI=1S/C20H19F3O4/c1-2-3-4-9-26-19(24)14-5-7-15(8-6-14)20(25)27-12-13-10-16(21
InchiKey:	APQYGBSGDRTZAK-UHFFFAOYSA-N
Formula:	C20H19F3O4
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCc2cc(F)c(F)c(F)c2)cc1
Mol. weight [g/mol]:	380.36

## Physical Properties

Property code	Value	Unit	Source
gf	-748.45	kJ/mol	Joback Method
hf	-1106.88	kJ/mol	Joback Method
hfus	48.90	kJ/mol	Joback Method
hvap	83.17	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	4.808		Crippen Method
mvol	265.330	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	2966.00		NIST Webbook
rinpol	2966.00		NIST Webbook
tb	880.67	K	Joback Method
tc	1090.49	K	Joback Method
tf	564.17	K	Joback Method
vc	1.042	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.91	J/mol×K	880.67	Joback Method
cpg	812.49	J/mol×K	915.64	Joback Method
cpg	823.93	J/mol×K	950.61	Joback Method
cpg	834.25	J/mol×K	985.58	Joback Method
cpg	843.47	J/mol×K	1020.55	Joback Method
cpg	851.62	J/mol×K	1055.52	Joback Method
cpg	858.70	J/mol×K	1090.49	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=U382891&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382891&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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