

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

Inchi:	InChI=1S/C19H17F3O4/c1-11(2)9-25-18(23)13-3-5-14(6-4-13)19(24)26-10-12-7-15(20)1
InchiKey:	DAPKOUAEZHAQKQ-UHFFFAOYSA-N
Formula:	C19H17F3O4
SMILES:	CC(C)COC(=O)c1ccc(C(=O)OCc2cc(F)c(F)c(F)c2)cc1
Mol. weight [g/mol]:	366.33

## Physical Properties

Property code	Value	Unit	Source
gf	-759.31	kJ/mol	Joback Method
hf	-1091.52	kJ/mol	Joback Method
hfus	42.78	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.274		Crippen Method
mcvol	251.240	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	857.35	K	Joback Method
tc	1069.18	K	Joback Method
tf	537.90	K	Joback Method
vc	0.980	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.57	J/mol×K	857.35	Joback Method
cpg	756.04	J/mol×K	892.66	Joback Method
cpg	767.39	J/mol×K	927.96	Joback Method
cpg	777.63	J/mol×K	963.27	Joback Method
cpg	786.78	J/mol×K	998.57	Joback Method
cpg	794.86	J/mol×K	1033.88	Joback Method
cpg	801.87	J/mol×K	1069.18	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=U382923&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382923&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>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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