

# Terephthalic acid, ethyl 2,3,5-trifluorobenzyl ester

Inchi:	InChI=1S/C17H13F3O4/c1-2-23-16(21)10-3-5-11(6-4-10)17(22)24-9-12-7-13(18)8-14(19)
InchiKey:	ISACACVNIOHQBB-UHFFFAOYSA-N
Formula:	C17H13F3O4
SMILES:	CCOC(=O)c1ccc(C(=O)OCc2cc(F)cc(F)c2F)cc1
Mol. weight [g/mol]:	338.28

## Physical Properties

Property code	Value	Unit	Source
gf	-773.71	kJ/mol	Joback Method
hf	-1044.96	kJ/mol	Joback Method
hfus	41.13	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.638		Crippen Method
mvol	223.060	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	2356.00		NIST Webbook
rinpol	2356.00		NIST Webbook
tb	812.03	K	Joback Method
tc	1023.37	K	Joback Method
tf	530.36	K	Joback Method
vc	0.874	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.67	J/molxK	812.03	Joback Method
cpg	643.52	J/molxK	847.25	Joback Method
cpg	654.37	J/molxK	882.48	Joback Method
cpg	664.23	J/molxK	917.70	Joback Method
cpg	673.09	J/molxK	952.92	Joback Method
cpg	680.98	J/molxK	988.14	Joback Method
cpg	687.89	J/molxK	1023.37	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=U416029&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416029&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>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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