

# Terephthalic acid, heptyl 2,2,2-trifluoroethyl ester

Inchi:	InChI=1S/C17H21F3O4/c1-2-3-4-5-6-11-23-15(21)13-7-9-14(10-8-13)16(22)24-12-17(18)
InchiKey:	HQYWIIKVBZXPAPZ-UHFFFAOYSA-N
Formula:	C17H21F3O4
SMILES:	CCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)F)cc1
Mol. weight [g/mol]:	346.34

## Physical Properties

Property code	Value	Unit	Source
gf	-854.39	kJ/mol	Joback Method
hf	-1255.83	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.533		Crippen Method
mvol	246.820	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	767.18	K	Joback Method
tc	957.59	K	Joback Method
tf	468.80	K	Joback Method
vc	0.971	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.19	J/molxK	767.18	Joback Method
cpg	743.32	J/molxK	798.92	Joback Method
cpg	756.53	J/molxK	830.65	Joback Method
cpg	768.84	J/molxK	862.39	Joback Method
cpg	780.28	J/molxK	894.12	Joback Method
cpg	790.87	J/molxK	925.86	Joback Method
cpg	800.66	J/molxK	957.59	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=U383042&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383042&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

Latest version available from:

<https://www.cheméo.com/cid/115-152-5/Terephthalic-acid-heptyl-2-2-2-trifluoroethyl-ester.pdf>

Generated by Cheméo on 2024-04-28 21:48:21.506450493 +0000 UTC m=+16630150.427027806.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.