

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

<b>Inchi:</b>	InChI=1S/C16H19F3O4/c1-2-3-4-5-10-22-14(20)12-6-8-13(9-7-12)15(21)23-11-16(17,18)
<b>InchiKey:</b>	ZWKVLKMLKCYPG-UHFFFAOYSA-N
<b>Formula:</b>	C16H19F3O4
<b>SMILES:</b>	CCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	332.31

## Physical Properties

Property code	Value	Unit	Source
gf	-862.81	kJ/mol	Joback Method
hf	-1235.19	kJ/mol	Joback Method
hfus	38.25	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.143		Crippen Method
mvol	232.730	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook
tb	744.30	K	Joback Method
tc	934.97	K	Joback Method
tf	457.53	K	Joback Method
vc	0.914	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.84	J/molxK	744.30	Joback Method
cpg	687.63	J/molxK	776.08	Joback Method
cpg	700.53	J/molxK	807.86	Joback Method
cpg	712.55	J/molxK	839.63	Joback Method
cpg	723.74	J/molxK	871.41	Joback Method
cpg	734.10	J/molxK	903.19	Joback Method
cpg	743.68	J/molxK	934.97	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U383041&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383041&amp;Units=SI</a>
<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.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>

# 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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