

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

Inchi:	InChI=1S/C19H25F3O4/c1-2-3-4-5-6-7-8-13-25-17(23)15-9-11-16(12-10-15)18(24)26-14
InchiKey:	WPOFGPQHIIKISJ-UHFFFAOYSA-N
Formula:	C19H25F3O4
SMILES:	CCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)F)cc1
Mol. weight [g/mol]:	374.39

## Physical Properties

Property code	Value	Unit	Source
gf	-837.55	kJ/mol	Joback Method
hf	-1297.11	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.313		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	812.94	K	Joback Method
tc	1004.64	K	Joback Method
tf	491.34	K	Joback Method
vc	1.083	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.80	J/molxK	812.94	Joback Method
cpg	857.56	J/molxK	844.89	Joback Method
cpg	871.33	J/molxK	876.84	Joback Method
cpg	884.14	J/molxK	908.79	Joback Method
cpg	896.01	J/molxK	940.74	Joback Method
cpg	907.00	J/molxK	972.69	Joback Method
cpg	917.13	J/molxK	1004.64	Joback Method

# Sources

<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=U383044&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383044&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>

# 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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