

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

<b>Inchi:</b>	InChI=1S/C21H21F3O4/c1-2-3-4-5-10-27-20(25)15-6-8-16(9-7-15)21(26)28-13-14-11-17
<b>InchiKey:</b>	LYYOLHYPWYHKTI-UHFFFAOYSA-N
<b>Formula:</b>	C21H21F3O4
<b>SMILES:</b>	CCCCCOC(=O)c1ccc(C(=O)OCc2cc(F)c(F)c(F)c2)cc1
<b>Mol. weight [g/mol]:</b>	394.38

## Physical Properties

Property code	Value	Unit	Source
gf	-740.03	kJ/mol	Joback Method
hf	-1127.52	kJ/mol	Joback Method
hfus	51.49	kJ/mol	Joback Method
hvap	85.40	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.198		Crippen Method
mvol	279.420	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	3066.00		NIST Webbook
rinpol	3066.00		NIST Webbook
tb	903.55	K	Joback Method
tc	1114.31	K	Joback Method
tf	575.44	K	Joback Method
vc	1.097	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.56	J/mol×K	903.55	Joback Method
cpg	870.32	J/mol×K	938.68	Joback Method
cpg	881.90	J/mol×K	973.80	Joback Method
cpg	892.31	J/mol×K	1008.93	Joback Method
cpg	901.59	J/mol×K	1044.06	Joback Method
cpg	909.74	J/mol×K	1079.18	Joback Method
cpg	916.79	J/mol×K	1114.31	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.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=U382890&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382890&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

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