

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

<b>Inchi:</b>	InChI=1S/C22H23F3O4/c1-2-3-4-5-6-11-28-21(26)16-7-9-17(10-8-16)22(27)29-14-15-12
<b>InchiKey:</b>	PHCZCZVXJHPLIY-UHFFFAOYSA-N
<b>Formula:</b>	C22H23F3O4
<b>SMILES:</b>	CCCCCCCOC(=O)c1ccc(C(=O)OCc2cc(F)c(F)c(F)c2)cc1
<b>Mol. weight [g/mol]:</b>	408.41

## Physical Properties

Property code	Value	Unit	Source
gf	-731.61	kJ/mol	Joback Method
hf	-1148.16	kJ/mol	Joback Method
hfus	54.08	kJ/mol	Joback Method
hvap	87.63	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	5.588		Crippen Method
mcvol	293.510	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
rinpol	3166.00		NIST Webbook
rinpol	3166.00		NIST Webbook
tb	926.43	K	Joback Method
tc	1138.93	K	Joback Method
tf	586.71	K	Joback Method
vc	1.153	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.88	J/mol×K	926.43	Joback Method
cpg	928.82	J/mol×K	961.85	Joback Method
cpg	940.51	J/mol×K	997.26	Joback Method
cpg	950.99	J/mol×K	1032.68	Joback Method
cpg	960.28	J/mol×K	1068.10	Joback Method
cpg	968.41	J/mol×K	1103.52	Joback Method
cpg	975.39	J/mol×K	1138.93	Joback Method

# Sources

<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=U382888&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382888&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvpap:</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>rinppl:</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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