

# Terephthalic acid, 2-fluoro-6-(trifluoromethyl)benzyl hexyl ester

Inchi:	InChI=1S/C22H22F4O4/c1-2-3-4-5-13-29-20(27)15-9-11-16(12-10-15)21(28)30-14-17-18
InchiKey:	SQSDPDIROVSCDN-UHFFFAOYSA-N
Formula:	C22H22F4O4
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCc2c(F)cccc2C(F)(F)F)cc1
Mol. weight [g/mol]:	426.40

## Physical Properties

Property code	Value	Unit	Source
gf	-913.95	kJ/mol	Joback Method
hf	-1341.55	kJ/mol	Joback Method
hfus	50.13	kJ/mol	Joback Method
hvap	84.85	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	5.939		Crippen Method
mvol	295.280	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	917.49	K	Joback Method
tc	1129.18	K	Joback Method
tf	577.20	K	Joback Method
vc	1.161	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.81	J/molxK	917.49	Joback Method
cpg	937.60	J/molxK	952.77	Joback Method
cpg	949.25	J/molxK	988.05	Joback Method
cpg	959.81	J/molxK	1023.33	Joback Method
cpg	969.33	J/molxK	1058.62	Joback Method
cpg	977.86	J/molxK	1093.90	Joback Method
cpg	985.44	J/molxK	1129.18	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=U382947&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382947&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>hvac:</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>rlnol:</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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