

# Terephthalic acid, heptyl 1-(pentafluorophenyl)ethyl ester

Inchi:	InChI=1S/C23H23F5O4/c1-3-4-5-6-7-12-31-22(29)14-8-10-15(11-9-14)23(30)32-13(2)16
InchiKey:	LNFVSFQOPMBOEL-UHFFFAOYSA-N
Formula:	C23H23F5O4
SMILES:	CCCCCCCOC(=O)c1ccc(C(=O)OC(C)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]:	458.42

## Physical Properties

Property code	Value	Unit	Source
gf	-1134.51	kJ/mol	Joback Method
hf	-1589.24	kJ/mol	Joback Method
hfus	58.52	kJ/mol	Joback Method
hvap	89.16	kJ/mol	Joback Method
log10ws	-8.62		Crippen Method
logp	6.427		Crippen Method
mvol	311.140	ml/mol	McGowan Method
pc	1126.83	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	957.37	K	Joback Method
tc	1172.30	K	Joback Method
tf	609.20	K	Joback Method
vc	1.240	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.89	J/molxK	957.37	Joback Method
cpg	999.34	J/molxK	993.19	Joback Method
cpg	1010.45	J/molxK	1029.01	Joback Method
cpg	1020.23	J/molxK	1064.84	Joback Method
cpg	1028.71	J/molxK	1100.66	Joback Method
cpg	1035.89	J/molxK	1136.48	Joback Method
cpg	1041.81	J/molxK	1172.30	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=U416059&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416059&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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