

# Phthalic acid, heptyl 4-trifluoromethoxybenzyl ester

Inchi:	InChI=1S/C23H25F3O5/c1-2-3-4-5-8-15-29-21(27)19-9-6-7-10-20(19)22(28)30-16-17-11
InchiKey:	SMTAMVWQWSETEC-UHFFFAOYSA-N
Formula:	C23H25F3O5
SMILES:	CCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	438.44

## Physical Properties

Property code	Value	Unit	Source
gf	-806.09	kJ/mol	Joback Method
hf	-1286.83	kJ/mol	Joback Method
hfus	51.22	kJ/mol	Joback Method
hvap	89.64	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.069		Crippen Method
mcvol	313.470	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	958.54	K	Joback Method
tc	1176.69	K	Joback Method
tf	597.59	K	Joback Method
vc	1.216	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.68	J/molxK	958.54	Joback Method
cpg	1017.34	J/molxK	994.90	Joback Method
cpg	1028.68	J/molxK	1031.26	Joback Method
cpg	1038.75	J/molxK	1067.62	Joback Method
cpg	1047.59	J/molxK	1103.97	Joback Method
cpg	1055.27	J/molxK	1140.33	Joback Method
cpg	1061.82	J/molxK	1176.69	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=U377689&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377689&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>
<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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