

# 6-Fluoro-3-trifluoromethylbenzoic acid, 4-isopropylphenyl ester

<b>Other names:</b>	6-Fluoro-3-trifluorobenzoic acid, 4-isopropylphenyl ester
<b>Inchi:</b>	InChI=1S/C17H14F4O2/c1-10(2)11-3-6-13(7-4-11)23-16(22)14-9-12(17(19,20)21)5-8-15
<b>InchiKey:</b>	XVUNPYRVBMYIPV-UHFFFAOYSA-N
<b>Formula:</b>	C17H14F4O2
<b>SMILES:</b>	CC(C)c1ccc(OC(=O)c2cc(C(F)(F)F)ccc2F)cc1
<b>Mol. weight [g/mol]:</b>	326.29

## Physical Properties

Property code	Value	Unit	Source
gf	-724.57	kJ/mol	Joback Method
hf	-998.83	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.187		Crippen Method
mcvol	217.390	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1899.00		NIST Webbook
rinpol	1899.00		NIST Webbook
tb	726.36	K	Joback Method
tc	936.57	K	Joback Method
tf	433.69	K	Joback Method
vc	0.851	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.82	J/molxK	726.36	Joback Method
cpg	617.80	J/molxK	761.39	Joback Method
cpg	630.73	J/molxK	796.43	Joback Method
cpg	642.68	J/molxK	831.46	Joback Method
cpg	653.70	J/molxK	866.50	Joback Method
cpg	663.83	J/molxK	901.53	Joback Method
cpg	673.13	J/molxK	936.57	Joback Method

# Sources

<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=U343788&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343788&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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