

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

<b>Other names:</b>	6-Fluoro-3-trifluorobenzoic acid, 3,4-dimethylphenyl ester
<b>Inchi:</b>	InChI=1S/C16H12F4O2/c1-9-3-5-12(7-10(9)2)22-15(21)13-8-11(16(18,19)20)4-6-14(13)
<b>InchiKey:</b>	KMPGPJJZJIXFEV-UHFFFAOYSA-N
<b>Formula:</b>	C16H12F4O2
<b>SMILES:</b>	<chem>Cc1ccc(OC(=O)c2cc(C(F)(F)F)ccc2F)cc1C</chem>
<b>Mol. weight [g/mol]:</b>	312.26

## Physical Properties

Property code	Value	Unit	Source
gf	-740.18	kJ/mol	Joback Method
hf	-984.38	kJ/mol	Joback Method
hfus	31.42	kJ/mol	Joback Method
hvap	63.00	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.681		Crippen Method
mcvol	203.300	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	708.90	K	Joback Method
tc	919.14	K	Joback Method
tf	449.94	K	Joback Method
vc	0.800	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.34	J/molxK	708.90	Joback Method
cpg	562.56	J/molxK	743.94	Joback Method
cpg	574.83	J/molxK	778.98	Joback Method
cpg	586.18	J/molxK	814.02	Joback Method
cpg	596.66	J/molxK	849.06	Joback Method
cpg	606.31	J/molxK	884.10	Joback Method
cpg	615.18	J/molxK	919.14	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=U343786&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343786&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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