

# 3-Fluoro-4-trifluoromethylbenzoic acid, 4-cyanophenyl ester

<b>Inchi:</b>	InChI=1S/C15H7F4NO2/c16-13-7-10(3-6-12(13)15(17,18)19)14(21)22-11-4-1-9(8-20)2-5
<b>InchiKey:</b>	VYNHUXCJIDEODH-UHFFFAOYSA-N
<b>Formula:</b>	C15H7F4NO2
<b>SMILES:</b>	N#Cc1ccc(OC(=O)c2ccc(C(F)(F)F)c(F)c2)cc1
<b>Mol. weight [g/mol]:</b>	309.22

## Physical Properties

Property code	Value	Unit	Source
gf	-605.79	kJ/mol	Joback Method
hf	-787.39	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.935		Crippen Method
mvol	190.590	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1983.00		NIST Webbook
rinpol	1983.00		NIST Webbook
tb	783.12	K	Joback Method
tc	1007.15	K	Joback Method
tf	491.14	K	Joback Method
vc	0.770	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.42	J/molxK	783.12	Joback Method
cpg	525.19	J/molxK	820.46	Joback Method
cpg	534.08	J/molxK	857.80	Joback Method
cpg	542.14	J/molxK	895.13	Joback Method
cpg	549.42	J/molxK	932.47	Joback Method
cpg	555.97	J/molxK	969.81	Joback Method
cpg	561.84	J/molxK	1007.15	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>
<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=U357945&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357945&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>

# 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>hvp:</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>rinp:</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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