

# 2-Fluoro-3-trifluoromethylbenzoic acid, 4-benzyloxyphenyl ester

**Inchi:** InChI=1S/C21H14F4O3/c22-19-17(7-4-8-18(19)21(23,24)25)20(26)28-16-11-9-15(10-12)  
**InchiKey:** UHJLUJULWCGDRF-UHFFFAOYSA-N  
**Formula:** C21H14F4O3  
**SMILES:** O=C(Oc1ccc(OCc2ccccc2)cc1)c1cccc(C(F)(F)F)c1F  
**Mol. weight [g/mol]:** 390.33

## Physical Properties

Property code	Value	Unit	Source
gf	-681.04	kJ/mol	Joback Method
hf	-971.80	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.643		Crippen Method
mcvol	255.860	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	867.42	K	Joback Method
tc	1094.88	K	Joback Method
tf	542.42	K	Joback Method
vc	0.991	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.82	J/mol×K	867.42	Joback Method
cpg	768.15	J/mol×K	905.33	Joback Method
cpg	779.27	J/mol×K	943.24	Joback Method
cpg	789.25	J/mol×K	981.15	Joback Method
cpg	798.16	J/mol×K	1019.06	Joback Method
cpg	806.08	J/mol×K	1056.97	Joback Method
cpg	813.07	J/mol×K	1094.88	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=U357654&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357654&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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