

# 4-Fluoro-2-trifluoromethylbenzoic acid, 2-ethoxyethyl ester

<b>Inchi:</b>	InChI=1S/C12H12F4O3/c1-2-18-5-6-19-11(17)9-4-3-8(13)7-10(9)12(14,15)16/h3-4,7H,2,
<b>InchiKey:</b>	WGXMVSVYPGCVMQ-UHFFFAOYSA-N
<b>Formula:</b>	C12H12F4O3
<b>SMILES:</b>	CCOCCOC(=O)c1ccc(F)cc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	280.22

## Physical Properties

Property code	Value	Unit	Source
gf	-972.01	kJ/mol	Joback Method
hf	-1247.63	kJ/mol	Joback Method
hfus	28.98	kJ/mol	Joback Method
hvap	52.91	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.038		Crippen Method
mcvol	176.570	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	603.16	K	Joback Method
tc	785.63	K	Joback Method
tf	375.63	K	Joback Method
vc	0.703	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.68	J/mol×K	603.16	Joback Method
cpg	467.25	J/mol×K	633.57	Joback Method
cpg	479.14	J/mol×K	663.98	Joback Method
cpg	490.36	J/mol×K	694.39	Joback Method
cpg	500.94	J/mol×K	724.80	Joback Method
cpg	510.89	J/mol×K	755.22	Joback Method
cpg	520.21	J/mol×K	785.63	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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=U343767&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343767&amp;Units=SI</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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