

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

Inchi:	InChI=1S/C12H12F4O2/c1-2-3-6-18-11(17)8-4-5-10(13)9(7-8)12(14,15)16/h4-5,7H,2-3,6
InchiKey:	POOZQODHGAEKNS-UHFFFAOYSA-N
Formula:	C12H12F4O2
SMILES:	CCCCOC(=O)c1ccc(F)c(C(F)(F)F)c1
Mol. weight [g/mol]:	264.22

## Physical Properties

Property code	Value	Unit	Source
gf	-867.01	kJ/mol	Joback Method
hf	-1115.41	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	50.50	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.801		Crippen Method
mcvol	170.700	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1317.00		NIST Webbook
rinpol	1317.00		NIST Webbook
tb	580.74	K	Joback Method
tc	764.11	K	Joback Method
tf	353.40	K	Joback Method
vc	0.684	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.48	J/mol×K	580.74	Joback Method
cpg	442.29	J/mol×K	611.30	Joback Method
cpg	454.38	J/mol×K	641.86	Joback Method
cpg	465.79	J/mol×K	672.43	Joback Method
cpg	476.53	J/mol×K	702.99	Joback Method
cpg	486.63	J/mol×K	733.55	Joback Method
cpg	496.11	J/mol×K	764.11	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=U338915&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338915&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>

# 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>rlnol:</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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