

# 5-Amino-2-methoxyphenol, O,N-bis(trifluoroacetyl)-

Inchi:	InChI=1S/C11H7F6NO4/c1-21-6-3-2-5(18-8(19)10(12,13)14)4-7(6)22-9(20)11(15,16)17/
InchiKey:	NIBNRKHLJRJMO-UHFFFAOYSA-N
Formula:	C11H7F6NO4
SMILES:	COc1ccc(N=C(O)C(F)(F)F)cc1OC(=O)C(F)(F)F
Mol. weight [g/mol]:	331.17

# Physical Properties

Property code	Value	Unit	Source
hf	-1707.76	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.313		Crippen Method
mcvol	177.570	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1481.00		NIST Webbook
tb	744.33	K	Joback Method
tc	933.02	K	Joback Method

## Sources

<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.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/cqi/cbook.cqi?ID=U374874&amp;Units=SI">http://webbook.nist.gov/cqi/cbook.cqi?ID=U374874&amp;Units=SI</a>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** 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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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