

# But-2-enamide, N-(2-fluorophenyl)-3-methyl-

<b>Inchi:</b>	InChI=1S/C11H12FNO/c1-8(2)7-11(14)13-10-6-4-3-5-9(10)12/h3-7H,1-2H3,(H,13,14)
<b>InchiKey:</b>	RMMBRAUAKCYSAN-UHFFFAOYSA-N
<b>Formula:</b>	C11H12FNO
<b>SMILES:</b>	CC(C)=CC(O)=Nc1ccccc1F
<b>Mol. weight [g/mol]:</b>	193.22

## Physical Properties

Property code	Value	Unit	Source
hf	-213.79	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.380		Crippen Method
mcvol	151.110	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1549.00		NIST Webbook
rinpol	1549.00		NIST Webbook
tb	654.79	K	Joback Method
tc	865.74	K	Joback Method

## Sources

<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=U308234&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308234&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.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>

## Legend

<b>hf:</b>	Enthalpy of formation 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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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