

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

Inchi:	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)
InchiKey:	RMMBRAUAKCYSAN-UHFFFAOYSA-N
Formula:	C11H12FNO
SMILES:	CC(C)=CC(O)=Nc1ccccc1F
Mol. weight [g/mol]:	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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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