

# Urea, 1,1'-p-phenylenebis[3-(2-fluoroethyl)-3-nitroso-

**Inchi:** InChI=1S/C12H14F2N6O4/c13-5-7-19(17-23)11(21)15-9-1-2-10(4-3-9)16-12(22)20(18-2  
**InchiKey:** PIRRAGAWVKRMAO-UHFFFAOYSA-N  
**Formula:** C12H14F2N6O4  
**SMILES:** O=NN(CCF)C(=O)Nc1ccc(NC(=O)N(CCF)N=O)cc1  
**Mol. weight [g/mol]:** 344.27  
**CAS:** 116277-65-7

## Physical Properties

Property code	Value	Unit	Source
hf	-777.71	kJ/mol	Joback Method
hvap	92.25	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.656		Crippen Method
mcvol	225.880	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
tb	863.92	K	Joback Method
tc	1065.00	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116277657&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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