

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

Inchi:	InChI=1S/C12H16N6O6/c19-7-5-17(15-23)11(21)13-9-1-2-10(4-3-9)14-12(22)18(16-24)6
InchiKey:	HMOWMQJSDDXBLW-UHFFFAOYSA-N
Formula:	C12H16N6O6
SMILES:	O=NN(CCO)C(=O)Nc1ccc(NC(=O)N(CCO)N=O)cc1
Mol. weight [g/mol]:	340.29
CAS:	116401-09-3

## Physical Properties

Property code	Value	Unit	Source
hf	-689.95	kJ/mol	Joback Method
hvap	127.25	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	0.702		Crippen Method
mcvol	234.080	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	1049.74	K	Joback Method
tc	1289.30	K	Joback Method

## Sources

**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>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401093&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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<https://www.chemeo.com/cid/94-011-5/Urea-1-1-p-phenylenebis-3-2-hydroxyethyl-3-nitroso.pdf>

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