

# Isocarbamid

<b>Other names:</b>	1-Imidazolidinecarboxamide, N-(2-methylpropyl)-2-oxo- 1-Imidazolidinecarboxamide, N-isobutyl-2-oxo- 1-Isobutylcarbamoyl-imidazolin-2-one Azolamide BAY 94871 Imidazolidin-2-on-1-carbonsaeure-isobutylamid Imidazolin-2-one, 1-isobutylcarbamoyl- Imizolamid Isocarbamide Isolamid MNF 166 Merpelan AZ N-Isobutyl-2-oxo-1-imidazolidinecarboxamide N-isobutyl-2-oxoimidazolidine-1-carboxamide Ozolamid
<b>Inchi:</b>	InChI=1S/C8H15N3O2/c1-6(2)5-10-8(13)11-4-3-9-7(11)12/h6H,3-5H2,1-2H3,(H,9,12)(H,
<b>InchiKey:</b>	SBYAVOHNDJTVPA-UHFFFAOYSA-N
<b>Formula:</b>	C8H15N3O2
<b>SMILES:</b>	CC(C)CNC(=O)N1CCNC1=O
<b>Mol. weight [g/mol]:</b>	185.22
<b>CAS:</b>	30979-48-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Aqueous Solubility Prediction Method
log10ws	-2.15		Estimated Solubility Method
logp	0.377		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
tf	368.65	K	Aqueous Solubility Prediction Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C30979487&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>  
**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

## Legend

**log<sub>10</sub>w<sub>s</sub>:** Log<sub>10</sub> of Water solubility in mol/l  
**log<sub>p</sub>:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**tf:** Normal melting (fusion) point

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