

# Buprofezin

**Other names:**

(Z)-2-(tert-butylimino)-3-isopropyl-5-phenyl-1,3,5-thiadiazinan-4-one  
2-((1,1-Dimethylethyl)imino)tetrahydro-3-(1-methylethyl)-5-phenyl-4H-1,3,5-thiadiazin-4-one  
2-tert-Butylimino-3-isopropyl-5-phenyl-1,3,5-thiadiazinan-4-one  
2-tert-Butylimino-3-isopropyl-5-phenyl-3,4,5,6-tetrahydro-2H-1,3,5-thiadiazin-4-one  
2-tert-Butylimino-3-isopropyl-5-phenylperhydro-1,3,5-thiadiazinan-4-one  
4H-1,3,5-Thiadiazin-4-one,  
2-((1,1-dimethylethyl)imino)tetrahydro-3-(1-methylethyl)-5-phenyl-  
Applaud  
Buprofezine  
NNI 750  
PP618

**Inchi:** InChI=1S/C16H23N3OS/c1-12(2)19-14(17-16(3,4)5)21-11-18(15(19)20)13-9-7-6-8-10-13  
**InchiKey:** PRLVTUNWOQKEAI-UHFFFAOYSA-N  
**Formula:** C16H23N3OS  
**SMILES:** CC(C)N1C(=O)N(c2ccccc2)CSC1=NC(C)(C)C  
**Mol. weight [g/mol]:** 305.44  
**CAS:** 69327-76-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	4.182		Crippen Method
mcvol	245.240	ml/mol	McGowan Method
rinpol	2201.00		NIST Webbook
rinpol	2229.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2205.00		NIST Webbook
rinpol	2204.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2229.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2219.00		NIST Webbook
ripol	2999.00		NIST Webbook
ripol	2999.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C69327760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C69327760&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Solvent effect on solubility and preferential solvation analysis of Buprofezin in aqueous and organic solvents:	<a href="https://www.doi.org/10.1016/j.jct.2019.06.019">https://www.doi.org/10.1016/j.jct.2019.06.019</a>
Solubility Determination and Thermodynamic Modeling of Buprofezin in Aqueous and Organic Solvents:	<a href="https://www.doi.org/10.1021/acs.jced.8b01099">https://www.doi.org/10.1021/acs.jced.8b01099</a>
Thermodynamic Modeling of Buprofezin in Aqueous and Organic Solvents:	<a href="https://www.doi.org/10.1021/acs.jced.9b00172">https://www.doi.org/10.1021/acs.jced.9b00172</a>
Mixing Properties of Solutions: Equilibrium of the Buprofezin in Pure and Binary Organic Solvents:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tt:	Triple Point Temperature

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