

# 2-Imidazolidinone, 3-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-4-hydroxy-1-methyl-2-imidazolidinone

<b>Other names:</b>	3-(5-(1,1-Dimethylethyl)-1,3,4-thiadiazol-2-yl)-4-hydroxy-1-methyl-2-imidazolidinone 3-(5-tert-butylthiadiazol-2-yl)-4-hydroxy-1-methylimidazolidine-2-one Buthidazole Ravage VEL 5026
<b>Inchi:</b>	InChI=1S/C10H16N4O2S/c1-10(2,3)7-11-12-8(17-7)14-6(15)5-13(4)9(14)16/h6,15H,5H2
<b>InchiKey:</b>	SWMGXKSQWDSBKV-UHFFFAOYSA-N
<b>Formula:</b>	C10H16N4O2S
<b>SMILES:</b>	CN1CC(O)N(c2nnc(C(C)(C)C)s2)C1=O
<b>Mol. weight [g/mol]:</b>	256.32
<b>CAS:</b>	55511-98-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Aqueous Solubility Prediction Method
log10ws	-1.88		Estimated Solubility Method
logp	1.026		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
tf	410.42 ± 0.20	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.46	kJ/mol	408.90	NIST Webbook

## Sources

<b>Estimated Solubility Method:</b>	<a href="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</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55511983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55511983&amp;Units=SI</a>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

## Legend

<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tf:</b>	Normal melting (fusion) point

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