

# 3-Picrylamino-1,2,4-triazole

**Inchi:** InChI=1S/C8H5N7O6/c16-13(17)4-1-5(14(18)19)7(6(2-4)15(20)21)11-8-9-3-10-12-8/h1-3  
**InchiKey:** IRXQEVVGPQRIPA-UHFFFAOYSA-N  
**Formula:** C8H5N7O6  
**SMILES:** O=[N+]([O-])c1cc([N+](=O)[O-])c(Nc2nc[nH]n2)c([N+](=O)[O-])c1  
**Mol. weight [g/mol]:** 295.17  
**CAS:** 18212-12-9

## Physical Properties

Property code	Value	Unit	Source
chs	-4014.00 ± 2.00	kJ/mol	NIST Webbook
hfs	151.00 ± 4.00	kJ/mol	NIST Webbook
log10ws	-3.98		Crippen Method
logp	0.791		Crippen Method
mcvol	172.540	ml/mol	McGowan Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18212129&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**chs:** Standard solid enthalpy of combustion  
**hfs:** Solid phase enthalpy of formation at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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