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
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/ci990307l

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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