5,7-Dinitro-1-picrylbenzotrizole

Inchi: InChI=1S/C12H4N8O10/c21-16(22)5-1-7-11(8(2-5)18(25)26)15(14-13-7)12-9(19(27)28)3
InchiKey: SAWVDTHMLXLYJS-UHFFFAOYSA-N
Formula: C12H4N8O10
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(-n2nnc3cc([N+](=O)[O-])cc([N+](=O)[O-])c32)c([N+](=O)
Mol. weight [g/mol]: 420.21
CAS: 50892-90-5

Physical Properties

Property code	Value	Unit	Source
chs	-5594.00 ± 3.00	kJ/mol	NIST Webbook
hfs	300.00 ± 5.90	kJ/mol	NIST Webbook
log10ws	-7.71		Crippen Method
logp	1.962		Crippen Method
mcvol	234.300	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=C50892905&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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