2,6-Bis(picrylazo)-3,5-dinitropyridine

Inchi: InChI=1S/C17H5N13O16/c31-23(32)6-1-8(25(35)36)14(9(2-6)26(37)38)19-21-16-12(29(4
InchiKey: BBVWILOPQSPUHG-FLFKKZLDSA-N
Formula: C17H5N13O16
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(N=Nc2nc(N=Nc3c([N+](=O)[O-])cc([N+](=O)[O-])cc3[N+
Mol. weight [g/mol]: 647.30
CAS: 55106-96-2

Physical Properties

Property code	Value	Unit	Source
chs	-8021.60 ± 0.84	kJ/mol	NIST Webbook
hfs	617.10 ± 5.00	kJ/mol	NIST Webbook
log10ws	-10.53		Crippen Method
logp	5.178		Crippen Method
mcvol	359.770	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55106962&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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