

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(
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+](=O) [O-])nc2
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

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