2,4,5,7-Tetranitrocarbazole

Inchi: InChI=1S/C12H5N5O8/c18-14(19)5-1-7-11(9(3-5)16(22)23)12-8(13-7)2-6(15(20)21)4-10
InchiKey: VSMSIASZXNTHEN-UHFFFAOYSA-N
Formula: C12H5N5O8
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c2c(c1)[nH]c1cc([N+](=O)[O-])cc([N+](=O)[O-])c12
Mol. weight [g/mol]: 347.20
CAS: 28453-24-9

Physical Properties

Property code	Value	Unit	Source
chs	-5455.50 ± 5.40	kJ/mol	NIST Webbook
hfs	18.80 ± 5.40	kJ/mol	NIST Webbook
log10ws	-6.90		Crippen Method
logp	2.472		Crippen Method
mcvol	201.220	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28453249&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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