2,4-Dimethoxy-6-(2-fluoro-2,2-dinitroethoxy)-1,3,5

Inchi: InChI=1S/C7H8FN5O7/c1-18-4-9-5(19-2)11-6(10-4)20-3-7(8,12(14)15)13(16)17/h3H2,1-
InchiKey: XSDYWUHPATXNBR-UHFFFAOYSA-N
Formula: C7H8FN5O7
SMILES: COc1nc(OC)nc(OCC(F)([N+](=O)[O-])[N+](=O)[O-])n1
Mol. weight [g/mol]: 293.17
CAS: 100508-56-3

Physical Properties

Property code	Value	Unit	Source
chs	-3380.20 ± 1.00	kJ/mol	NIST Webbook
hfs	-697.10 ± 1.20	kJ/mol	NIST Webbook
log10ws	-2.67		Crippen Method
logp	-0.556		Crippen Method
mcvol	169.890	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100508563&Units=SI

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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