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

Inchi: InChI=1S/C8H7F2N7O11/c1-26-4-11-5(27-2-7(9,14(18)19)15(20)21)13-6(12-4)28-3-8(10
InchiKey: MWDAMNNZTWJXEP-UHFFFAOYSA-N
Formula: C8H7F2N7O11
SMILES: COc1nc(OCC(F)([N+](=O)[O-])[N+](=O)[O-])nc(OCC(F)([N+](=O)[O-])[N+](=O)[O-])n1
Mol. weight [g/mol]: 415.18
CAS: 100508-57-4

Physical Properties

Property code	Value	Unit	Source
chs	-3599.70 ± 2.30	kJ/mol	NIST Webbook
hfs	-907.70 ± 2.40	kJ/mol	NIST Webbook
log10ws	-4.21		Crippen Method
logp	-1.009		Crippen Method
mcvol	220.590	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=C100508574&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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