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

Inchi: InChI=1S/C9H6F3N9O15/c10-7(16(22)23,17(24)25)1-34-4-13-5(35-2-8(11,18(26)27)19(2
InchiKey: GJYPVHOKDDJFAH-UHFFFAOYSA-N
Formula: C9H6F3N9O15
SMILES: O=[N+]([O-])C(F)(COc1nc(OCC(F)([N+](=O)[O-])[N+](=O)[O-])nc(OCC(F)([N+](=O)[O-])[N
Mol. weight [g/mol]: 537.19
CAS: 28820-59-9

Physical Properties

Property code	Value	Unit	Source
chs	-3827.60 ± 1.20	kJ/mol	NIST Webbook
hfs	-1109.80 ± 1.50	kJ/mol	NIST Webbook
log10ws	-5.76		Crippen Method
logp	-1.462		Crippen Method
mcvol	271.290	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=C28820599&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

Latest version available from: