2,4,6-Triethoxy-1,3,5-triazine

Inchi: InChI=1S/C9H15N3O3/c1-4-13-7-10-8(14-5-2)12-9(11-7)15-6-3/h4-6H2,1-3H3
InchiKey: ZLKYBXDNXFQYDL-UHFFFAOYSA-N
Formula: C9H15N3O3
SMILES: CCOc1nc(OCC)nc(OCC)n1
Mol. weight [g/mol]: 213.23
CAS: 884-43-5

Physical Properties

Property code	Value	Unit	Source
chs	-5100.30 ± 1.40	kJ/mol	NIST Webbook
hfs	-585.00 ± 1.50	kJ/mol	NIST Webbook
log10ws	-1.48		Aqueous Solubility Prediction Method
logp	1.068		Crippen Method
mcvol	161.460	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=C884435&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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