N-Formylimidazole diethyl acetal

Inchi: InChI=1S/C8H14N2O2/c1-3-12-8(6-11-2)10-5-4-9-7-10/h4-5,7-8H,3,6H2,1-2H3
InchiKey: SXYWTJVFBWNDCA-UHFFFAOYSA-N
Formula: C8H14N2O2
SMILES: CCOC(COC)n1ccnc1
Mol. weight [g/mol]: 170.21
CAS: 61278-81-7

Physical Properties

Property code	Value	Unit	Source
hf	-255.30 ± 3.00	kJ/mol	NIST Webbook
hfl	-329.30 ± 2.80	kJ/mol	NIST Webbook
hvap	74.00 ± 1.20	kJ/mol	NIST Webbook
log10ws	-1.39		Crippen Method
logp	1.065		Crippen Method
mcvol	135.820	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=C61278817&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume