# Acetylimidazole diethyl acetal

**Inchi:** InChI=1S/C9H16N2O2/c1-4-12-9(3,13-5-2)11-7-6-10-8-11/h6-8H,4-5H2,1-3H3
**InchiKey:** WHHNCTBBIVAUTJ-UHFFFAOYSA-N
**Formula:** C9H16N2O2
**SMILES:** CCOC(C)(OCC)n1ccnc1
**Mol. weight [g/mol]:** 184.24
**CAS:** 111456-84-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -296.80 ± 2.30 | kJ/mol | NIST Webbook |
| hfl | -368.90 ± 2.00 | kJ/mol | NIST Webbook |
| hvap | 72.20 ± 1.20 | kJ/mol | NIST Webbook |
| log10ws | -2.01 | | Crippen Method |
| logp | 1.586 | | Crippen Method |
| mcvol | 149.910 | ml/mol | McGowan Method |

## Sources

**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=C111456849&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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