

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/ci9903071>

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

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