Furo[2,3,4-gh]pyrrolizin-2(2aH)-one, hexahydro-, (2a«alpha», 7a«alpha», 7b«alpha»)-

Other names: Furo[2,3,4-gh]pyrrolizin-2(2a«alpha»H)-one, 3,4,5,6,7,7a-hexahydro-(2a«alpha», 7a«alpha», 7b«alpha»)-; 1-Carboxypyrrolizidine-7-olide

Inchi: InChI=1S/C8H11NO2/c10-8-5-1-3-9-4-2-6(11-8)7(5)9/h5-7H,1-4H2

InchiKey: RYWDCLFOABOLBP-UHFFFAOYSA-N

Formula: C8H11NO2

SMILES: O=C1OC2CCN3CCC1C23

Mol. weight [g/mol]: 153.18

CAS: 25471-69-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.27		Crippen Method
logp	0.006		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
rinpol	1408.00		NIST Webbook
rinpol	1408.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25471696&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices