Pyrazine, 2-[2-(diethylamino)-ethyl]-

Inchi: InChI=1S/C10H17N3/c1-3-13(4-2)8-5-10-9-11-6-7-12-10/h6-7,9H,3-5,8H2,1-2H3
InchiKey: AZMKHGHSZCYFDN-UHFFFAOYSA-N
Formula: C10H17N3
SMILES: CCN(CC)CCc1cnccn1
Mol. weight [g/mol]: 179.26
CAS: 91140-68-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	1.361		Crippen Method
mcvol	157.940	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=C91140680&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume