

hexyl pyrazine

Other names: Pyrazine, hexyl-
Inchi: InChI=1S/C10H16N2/c1-2-3-4-5-6-10-9-11-7-8-12-10/h7-9H,2-6H2,1H3
InchiKey: LZQRFVUKPVNFJO-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CCCCCc1cnccn1
Mol. weight [g/mol]: 164.25
CAS: 28217-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.599		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1668.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C28217916&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

ripol: Polar retention indices

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