

Hygroline B/A

Inchi: InChI=1S/C8H17NO/c1-7(10)6-8-4-3-5-9(8)2/h7-8,10H,3-6H2,1-2H3/t7-,8-/m1/s1
InchiKey: CWMYODFAUAJKIV-HTQZYQBOSA-N
Formula: C8H17NO
SMILES: CC(O)CC1CCCN1C
Mol. weight [g/mol]: 143.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	0.852		Crippen Method
mcvol	128.570	ml/mol	McGowan Method
rinpol	1116.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1116.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=R570139&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/91-903-8/Hygroline-B-A.pdf>

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