

Ethane, 1,2-bis-(2-pyrazinyl)

Inchi: InChI=1S/C10H10N4/c1(9-7-11-3-5-13-9)2-10-8-12-4-6-14-10/h3-8H,1-2H2
InchiKey: DDDNWWSVGPACCT-UHFFFAOYSA-N
Formula: C10H10N4
SMILES: c1cnc(CCc2cnccn2)cn1
Mol. weight [g/mol]: 186.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	1.052		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
rinpol	1626.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R87996&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

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<https://www.chemeo.com/cid/85-969-3/Ethane-1-2-bis-2-pyrazinyl.pdf>

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