

5-METHYL-6,7-DIHYDRO-5H-CYCLOPENTAPYRAZINE

Other names:	5H-Cyclopentapyrazine, 6,7-dihydro-5-methyl- 5-Methyl-5H-cyclopenta[b]pyrazine, 6,7-dihydro 5-Methyl-6,7-dihydro-5H-cyclopenta[b]pyrazine 5-Methyl-(5H)-6,7-dihydrocyclo- pentapyrazine 5-Methyl-6,7-dihydro-(5H)-cyclopentapyrazine 5-Methyl -6,7-dihydrocyclopentapyrazine 6,7-Dihydro-5-methyl-5H-cyclopentapyrazine 5-methyl-dihydro-6,7-[5H]-cyclopenta[b]pyrazine
Inchi:	InChI=1S/C8H10N2/c1-6-2-3-7-8(6)10-5-4-9-7/h4-6H,2-3H2,1H3
InchiKey:	YZEFQPIMXZVPKP-UHFFFAOYSA-N
Formula:	C8H10N2
SMILES:	CC1CCc2nccnc21
Mol. weight [g/mol]:	134.18

Physical Properties

Property code	Value	Unit	Source
logp	1.526		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
rinpol	1158.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1163.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1667.00		NIST Webbook

ripol	1667.00	NIST Webbook
ripol	1594.00	NIST Webbook
ripol	1605.00	NIST Webbook
ripol	1603.00	NIST Webbook
ripol	1643.00	NIST Webbook
ripol	1630.00	NIST Webbook
ripol	1636.00	NIST Webbook
ripol	1643.00	NIST Webbook
ripol	1616.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23747480&Units=SI>

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

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

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices

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