

Retamine

Inchi: InChI=1S/C15H26N2O/c18-14-5-3-7-17-9-11-8-12(15(14)17)10-16-6-2-1-4-13(11)16/h11
InchiKey: JMXNBIDTNISOTA-UHFFFAOYSA-N
Formula: C15H26N2O
SMILES: OC1CCCN2CC3CC(CN4CCCCC34)C12
Mol. weight [g/mol]: 250.38
CAS: 2122-29-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	1.316		Crippen Method
mcvol	204.600	ml/mol	McGowan Method
rinpol	1970.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1980.00		NIST Webbook

Sources

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=C2122294&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/22-408-4/Retamine.pdf>

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