Panamine II

Inchi: InChI=1S/C20H33N3/c1-2-9-22-13-20-12-15(16(22)6-1)11-14-5-4-10-23(19(14)20)18-8-3
InchiKey: MRLGBUWOAFGOBH-SYRRFROPSA-N
Formula: C20H33N3
SMILES: C1CCN2CC34CC(CC5CCCN(C6CCCC3N6)C54)C2C1
Mol. weight [g/mol]: 315.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	2.813		Crippen Method
mcvol	257.440	ml/mol	McGowan Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R402789&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.