homopiptanthine

Inchi: InChI=1S/C21H35N3/c1-3-9-22-14-21-13-17(18(22)7-1)12-16-6-5-11-24(20(16)21)15-23-
InchiKey: GFDFZTFQPIBNSQ-XJPWDTPTSA-N
Formula: C21H35N3
SMILES: C1CCN2CC34CC(CC5CCCN(CN6CCCCC63)C54)C2C1
Mol. weight [g/mol]: 329.52
CAS: 38965-96-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.157		Crippen Method
mcvol	271.530	ml/mol	McGowan Method
rinpol	2590.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38965967&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

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