2,5-Bis(1-bromo-1-methylethyl)pyrazine

Inchi: InChI=1S/C10H14Br2N2/c1-9(2,11)7-5-14-8(6-13-7)10(3,4)12/h5-6H,1-4H3
InchiKey: MDOOVWSOSVQGOM-UHFFFAOYSA-N
Formula: C10H14Br2N2
SMILES: CC(C)(Br)c1cnc(C(C)(C)Br)cn1
Mol. weight [g/mol]: 322.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	3.737		Crippen Method
mcvol	182.960	ml/mol	McGowan Method
rinpol	1718.00		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=R412825&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices