2,3-Dimethyl-5-n-propylpyrazine

Other names: 2,3-Dimethyl-5-propylpyrazine
Inchi: InChI=1S/C9H14N2/c1-4-5-9-6-10-7(2)8(3)11-9/h6H,4-5H2,1-3H3
InchiKey: RHCYSZMTNWMCOO-UHFFFAOYSA-N
Formula: C9H14N2
SMILES: CCCc1cnc(C)c(C)n1
Mol. weight [g/mol]: 150.22
CAS: 32262-98-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.046		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1154.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1166.00		NIST Webbook
ripol	1500.00		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=C32262989&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

ripol: Polar retention indices