Pyrazine, (2-methylpentyl)-

Other names: 2-methyl pentyl pyrazine
Inchi: InChI=1S/C10H16N2/c1-3-4-9(2)7-10-8-11-5-6-12-10/h5-6,8-9H,3-4,7H2,1-2H3
InchiKey: UQDNAXJKOPOWKM-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CCCC(C)Cc1cnccn1
Mol. weight [g/mol]: 164.25
CAS: 107697-81-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.455		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1606.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107697814&Units=SI
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

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