Pyrazine, 2-(n-propyl)-

Other names: Propylpyrazine
2-Propylpyrazine
N-Propylpyrazine
Inchi: InChI=1S/C7H10N2/c1-2-3-7-6-8-4-5-9-7/h4-6H,2-3H2,1H3
InchiKey: DJLLTFRHLPVCEL-UHFFFAOYSA-N
Formula: C7H10N2
SMILES: CCCc1cnccn1
Mol. weight [g/mol]: 122.17
CAS: 18138-03-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	1.429		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
rinpol	1009.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	980.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1428.00		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=C18138039&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
ripol:	Polar retention indices