

2,3-Diethylpyrazine

Other names:	Pyrazine, 2,3-diethyl-
Inchi:	InChI=1S/C8H12N2/c1-3-7-8(4-2)10-6-5-9-7/h5-6H,3-4H2,1-2H3
InchiKey:	GZXXANJCCWGCSV-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CCc1nccnc1CC
Mol. weight [g/mol]:	136.19
CAS:	15707-24-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.601		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1106.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1449.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1431.00		NIST Webbook
tb	454.20	K	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=C15707241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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