

Pyrazine, 2,5-diethyl-

Other names:	2,5-Diethylpyrazine
Inchi:	InChI=1S/C8H12N2/c1-3-7-5-10-8(4-2)6-9-7/h5-6H,3-4H2,1-2H3
InchiKey:	WAVOLMBVDCRBGR-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CCc1cnc(CC)cn1
Mol. weight [g/mol]:	136.19
CAS:	13238-84-1

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	1091.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1077.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1443.00		NIST Webbook
ripol	1449.00		NIST Webbook
ripol	1456.00		NIST Webbook
ripol	1433.00		NIST Webbook

ripol	1463.00	NIST Webbook
ripol	1461.00	NIST Webbook
ripol	1492.00	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=C13238841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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