

Phenacyl pyrazine

Inchi:	InChI=1S/C12H10N2O/c15-12(10-4-2-1-3-5-10)8-11-9-13-6-7-14-11/h1-7,9H,8H2
InchiKey:	WUYTZBFFXRNJSB-UHFFFAOYSA-N
Formula:	C12H10N2O
SMILES:	O=C(Cc1cnccn1)c1cccc1
Mol. weight [g/mol]:	198.22
CAS:	40061-45-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	1.902		Crippen Method
mcvol	153.950	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40061458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/85-589-5/Phenacyl-pyrazine.pdf>

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