

Furan, 3-bromo-

Other names:	«beta»-Bromofuran 3-Bromofuran
Inchi:	InChI=1S/C4H3BrO/c5-4-1-2-6-3-4/h1-3H
InchiKey:	LXWLEQZDXOQZGW-UHFFFAOYSA-N
Formula:	C4H3BrO
SMILES:	Brc1ccoc1
Mol. weight [g/mol]:	146.97
CAS:	22037-28-1

Physical Properties

Property code	Value	Unit	Source
ie	9.14	eV	NIST Webbook
log10ws	-6.37		Crippen Method
logp	2.042		Crippen Method
mcvol	71.130	ml/mol	McGowan Method
tb	376.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22037281&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

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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