3-Furanmethanol

Other names: 3-Hydroxymethylfuran
furan-3-methanol
Inchi: InChI=1S/C5H6O2/c6-3-5-1-2-7-4-5/h1-2,4,6H,3H2
InchiKey: STJIISDMSMJQQK-UHFFFAOYSA-N
Formula: C5H6O2
SMILES: OCc1ccoc1
Mol. weight [g/mol]: 98.10
CAS: 4412-91-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	0.772		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
rinpol	835.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1684.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.70	K	2.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4412913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure