2,5-di-(Hydroxymethyl)furan

Inchi:	InChI=1S/C6H8O3/c7-3-5-1-2-6(4-8)9-5/h1-2,7-8H,3-4H2
InchiKey:	DSLRVRBSNLHVBH-UHFFFAOYSA-N
Formula:	C6H8O3
SMILES:	OCc1ccc(CO)o1
Mol. weight [g/mol]:	128.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	0.264		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R614898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices

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