

1-Cyclobutylethanol

Inchi:	InChI=1S/C6H12O/c1-5(7)6-3-2-4-6/h5-7H,2-4H2,1H3
InchiKey:	PFGPCAYJUYSJJS-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CC([O])C1CCC1
Mol. weight [g/mol]:	100.16
CAS:	38401-41-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.99		Crippen Method
logp	1.605		Crippen Method
mcvol	88.260	ml/mol	McGowan Method

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=C38401411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/55-788-7/1-Cyclobutylethanol.pdf>

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