

3-Thiopheneethanol

Other names:	2-(3-Thienyl)ethanol thiophene-3-ethanol
Inchi:	InChI=1S/C6H8OS/c7-3-1-6-2-4-8-5-6/h2,4-5,7H,1,3H2
InchiKey:	YYPNNBPPDFTQFX-UHFFFAOYSA-N
Formula:	C6H8OS
SMILES:	OCCc1ccsc1
Mol. weight [g/mol]:	128.19
CAS:	13781-67-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	1.283		Crippen Method
mcpvol	98.160	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.70	K	1.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13781674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tbrp:	Boiling point at reduced pressure

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