

2-Thenoylacetonitrile

Inchi:	InChI=1S/C7H5NOS/c8-4-3-6(9)7-2-1-5-10-7/h1-2,5H,3H2
InchiKey:	XWWUQBHVRILEPB-UHFFFAOYSA-N
Formula:	C7H5NOS
SMILES:	N#CCC(=O)c1cccs1
Mol. weight [g/mol]:	151.19
CAS:	33898-90-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	1.844		Crippen Method
mcvol	109.330	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33898907&Units=SI

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/12-996-3/2-Thenoylacetonitrile.pdf>

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