

2-Acetylthiazole

Other names:	Ethanone, 1-(2-thiazolyl)- Ketone, methyl 2-thiazolyl 1-(1,3-Thiazol-2-yl)ethanone 2-Acetylthiazol Thiazole, 2-acetyl 1-(2-Thiazolyl)ethanone Methyl 2-thiazolyl ketone 1-(thiazol-2-yl)ethan-1-one
Inchi:	InChI=1S/C5H5NOS/c1-4(7)5-6-2-3-8-5/h2-3H,1H3
InchiKey:	MOMFXATYAINJML-UHFFFAOYSA-N
Formula:	C5H5NOS
SMILES:	CC(=O)c1nccs1
Mol. weight [g/mol]:	127.16
CAS:	24295-03-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.65		Crippen Method
logp	1.346		Crippen Method
mcvol	89.750	ml/mol	McGowan Method
rinpol	979.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1038.00		NIST Webbook

rinpol	989.00	NIST Webbook
rinpol	989.00	NIST Webbook
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rinpol	1020.00	NIST Webbook
rinpol	1020.00	NIST Webbook
rinpol	1015.00	NIST Webbook
rinpol	1015.00	NIST Webbook
rinpol	1021.00	NIST Webbook
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ripol	1635.00	NIST Webbook
ripol	1634.00	NIST Webbook
ripol	1647.00	NIST Webbook
ripol	1661.00	NIST Webbook
ripol	1615.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.20	K	1.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24295032&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure

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