2-Propionyl thiazole

Other names:	2-Propanoyl-thiazole
	2-propionylthiazol
	Thiazole, 2-(1-oxopropyl)
	2-thiazolyl-1-propanone
	Thiazole, 2-propionyl-
	2-(1-propanonyl)thiazole
	1-(2-thiazolyl)-1-propanone
	1-Propanone, 1-(2-thiazolyl)-
	1-(1,3-thiazol-2-yl)propan-1-one
Inchi:	InChI=1S/C6H7NOS/c1-2-5(8)6-7-3-4-9-6/h3-4H,2H2,1H3
InchiKey:	TYRAENAWSLPSLW-UHFFFAOYSA-N
Formula:	C6H7NOS
SMILES:	CCC(=O)c1nccs1
Mol. weight [g/mol]:	141.19
CAS:	43039-98-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	1.736		Crippen Method
mcvol	103.840	ml/mol	McGowan Method
rinpol	1132.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1083.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1702.00		NIST Webbook

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=C43039981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices