

1-(2-Thienyl)-1-propanone

Other names:	2-Propionylthiophene Ethyl-2-thienylketone 1-Propanone, 1-(2-thienyl)- 1-thiophene-2-yl-propan-1-one 2-(1-propionyl)thiophene Thiophene, 2-propionyl 1 -(Thienyl)-1 -propanone 1-(2-Thienyl)propanone 1-(2-thienyl)propan-1-one
Inchi:	InChI=1S/C7H8OS/c1-2-6(8)7-4-3-5-9-7/h3-5H,2H2,1H3
InchiKey:	MFPZQZZWAMAHOY-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	CCC(=O)c1cccs1
Mol. weight [g/mol]:	140.20
CAS:	13679-75-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	2.341		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1181.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1181.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1842.00		NIST Webbook
ripol	1840.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	1.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure

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