2-ACETYL-3-METHYLTHIOPHENE

Other names:	1-(3-Methyl-2-thienyl)ethanone
	1-(3-methyl-2-thienyl)ethan-1-one
	3-methyl-2-acetylthiophene
	3-methyl-2-thienyl methyl ketone
	Ethanone, 1-(3-methyl-2-thienyl)-
	Thiophene, 2-acetyl-3-methyl
	thiophene, 2-acetyl-3-methyl-
Inchi:	InChI=1S/C7H8OS/c1-5-3-4-9-7(5)6(2)8/h3-4H,1-2H3
InchiKey:	YBJDKNXEWQSGEL-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	CC(=O)c1sccc1C
Mol. weight [g/mol]:	140.21

Physical Properties

Property code	Value	Unit	Source
hvap	57.10 ± 2.40	kJ/mol	NIST Webbook
ie	8.84	eV	Cheméo Relay (1.0)
logp	2.259		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1137.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1186.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1760.00		NIST Webbook
tb	484.44	K	Cheméo Relay (1.0)
tf	272.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hvapt	57.10	kJ/mol	298.15	Experimental thermochemical study of the three methyl substituted 2-acetylthiophene isomers

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Experimental thermochemical study of the three methyl substituted 2-acetylthiophene isomers:	https://www.doi.org/10.1016/j.jct.2008.03.008
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679726&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point