3-ACETYL-2,5-DIMETHYLTHIOPHENE

Other names:	2,5-dimethylthiophen-3-yl methyl ketone
	Dimethylthienylcetone
	Ethanone, 1-(2,5-dimethyl-3-thienyl)-
	Ketone, 2,5-dimethyl-3-thienyl methyl
Inchi:	InChI=1S/C8H10OS/c1-5-4-8(6(2)9)7(3)10-5/h4H,1-3H3
InchiKey:	PUSJAEJRDNPYKM-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	CC(=O)c1cc(C)sc1C
Mol. weight [g/mol]:	154.23

Physical Properties

Property code	Value	Unit	Source
hf	-143.34	kJ/mol	Cheméo Relay (1.0)
hvap	59.15	kJ/mol	Cheméo Relay (1.0)
logp	2.568		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
tb	499.07	K	Cheméo Relay (1.0)
tf	308.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	61.30	kJ/mol	298.15	Experimental study on the thermochemistry of 2,5-dimethylthiophene and its acetyl derivative

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Experimental study on the thermochemistry of 2,5-dimethylthiophene and its acetyl derivative:	https://www.doi.org/10.1016/j.jct.2008.04.005
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2530101&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point