3-Acetyl-2-methyl-5-phenylthiophene

Inchi: InChI=1S/C13H12OS/c1-9(14)12-8-13(15-10(12)2)11-6-4-3-5-7-11/h3-8H,1-2H3
InchiKey: GREAZYFTAJMZFD-UHFFFAOYSA-N
Formula: C13H12OS
SMILES: CC(=O)c1cc(-c2ccccc2)sc1C
Mol. weight [g/mol]: 216.30
CAS: 40932-63-6

Physical Properties

Property code	Value	Unit	Source
hsub	108.90 ± 0.40	kJ/mol	NIST Webbook
log10ws	-4.97		Crippen Method
logp	3.926		Crippen Method
mcvol	168.730	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	107.30 ± 0.40	kJ/mol	330.00	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=C40932636&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume