

2-Acetyl-5-bromothiophene

Other names:	5-Bromo-2-thienyl methyl ketone 5-Bromo 2-acetylthiophene Ethanone, 1-(5-bromo-2-thienyl)- Ketone, 5-bromo-2-thienyl methyl 1-(5-bromo-2-thienyl)ethan-1-one
Inchi:	InChI=1S/C6H5BrOS/c1-4(8)5-2-3-6(7)9-5/h2-3H,1H3
InchiKey:	IGBZCOWXSCWSHO-UHFFFAOYSA-N
Formula:	C6H5BrOS
SMILES:	CC(=O)c1ccc(Br)s1
Mol. weight [g/mol]:	205.07
CAS:	5370-25-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.713		Crippen Method
mcvol	111.360	ml/mol	McGowan Method
tf	367.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	0.50	NIST Webbook
tbrp	378.00	K	0.03	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=C5370252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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