2-Acetylbenzofuran

Other names:	1-(2-Benzofuranyl)ethanone
	1-(2-benzofuranyl)-1-ethanone
	2-Acetylbenzo[b]furan
	2-acetylcoumarone
	2-benzofuranyl methyl ketone
	Benzo(b)furan-2-yl methyl ketone
	Benzofuran-2-yl methyl ketone
	Ethanone, 1-(2-benzofuranyl)-
	Ketone, 2-benzofuranyl methyl
	NSC 23974
	NSC 28904
Inchi:	InChI=1S/C10H8O2/c1-7(11)10-6-8-4-2-3-5-9(8)12-10/h2-6H,1H3
InchiKey:	YUTFQTAITWWGFH-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	CC(=O)c1cc2ccccc2o1
Mol. weight [g/mol]:	160.17
CAS:	1646-26-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.67		Crippen Method
logp	2.635		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
tf	339.00	K	Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.70	K	0.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1646260&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives:	https://www.doi.org/10.1016/j.jct.2016.02.008

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