Benzofuran-2-carboxaldehyde

Other names:	2-Benzofurancarboxaldehyde
	Benzo[b]furan-2-carboxaldehyde
Inchi:	InChI=1S/C9H6O2/c10-6-8-5-7-3-1-2-4-9(7)11-8/h1-6H
InchiKey:	ADDZHRRCUWNSCS-UHFFFAOYSA-N
Formula:	C9H6O2
SMILES:	O=Cc1cc2ccccc2o1
Mol. weight [g/mol]:	146.14
CAS:	4265-16-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.25		Crippen Method
logp	2.245		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.00 ± 5.00	K	0.10	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=C4265161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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