Benzofuran-2-carboxylic acid

Other names:	2,3-benzofuran-2-carboxylic acid
	2-Benzofurancarboxylic acid
	2-Carboxybenzofuran
	Benzo[b]furan-2-carboxylic acid
	coumarilic acid
	coumarone-2-carboxylic acid
Inchi:	InChI=1S/C9H6O3/c10-9(11)8-5-6-3-1-2-4-7(6)12-8/h1-5H,(H,10,11)
InchiKey:	OFFSPAZVIVZPHU-UHFFFAOYSA-N
Formula:	C9H6O3
SMILES:	O=C(O)c1cc2ccccc2o1
Mol. weight [g/mol]:	162.14
CAS:	496-41-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.07		Crippen Method
logp	2.131		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
tb	585.70	K	NIST Webbook
tb	585.50 ± 2.50	K	NIST Webbook
tf	465.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhos	1340.00	kg/m3	298.15	Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C496413&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
rhos:	Solid Density
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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