

Thianaphthene-2-carboxylic acid

Other names:	benzo[b]thiophene-2-carboxylic acid benzothiophene-2-carboxylic acid
Inchi:	InChI=1S/C9H6O2S/c10-9(11)8-5-6-3-1-2-4-7(6)12-8/h1-5H,(H,10,11)
InchiKey:	DYSJMQABFPKAQM-UHFFFAOYSA-N
Formula:	C9H6O2S
SMILES:	O=C(O)c1cc2ccccc2s1
Mol. weight [g/mol]:	178.21
CAS:	6314-28-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	2.599		Crippen Method
mcvol	122.540	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhos	1490.00	kg/m3	298.15	Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6314289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives:	http://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

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