Benzp[b]thiophene-3-acetic acid

Other names:	Benzo[b]thiophene-3-acetic acid
	Acetic acid, 3-benzo(b)thienyl-
	3-Benzo(b)thienylacetic acid
	Benzp[b]thiophene-3-acetic acid
Inchi:	InChI=1S/C10H8O2S/c11-10(12)5-7-6-13-9-4-2-1-3-8(7)9/h1-4,6H,5H2,(H,11,12)
InchiKey:	VFZQJKXVHYZXMM-UHFFFAOYSA-N
Formula:	C10H8O2S
SMILES:	O=C(O)Cc1csc2ccccc12
Mol. weight [g/mol]:	192.24

Physical Properties

Property code	Value	Unit	Source
hvap	96.24	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-2.72		Cheméo Relay (1.0)
logp	2.528		Crippen Method
mcvol	136.630	ml/mol	McGowan Method
pc	4064.22	kPa	Cheméo Relay (1.0, beta)
tb	608.10	K	Cheméo Relay (1.0)
tf	417.56	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1131095&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point