Benzo[b]thiophene-4-ol, methylcarbamate

Other names:	Mobam
	Carbamic acid, methyl-, benzo[b]thien-4-yl ester
	Benzo[b]thien-4-yl methylcarbamate
	Mobam phenol
	Mobil MC-A-600
	MCA 600
	4-Benzothienyl methylcarbamate
	4-Benzothienylester kyseliny methylkarbaminove
	ENT-27041
	MOS-708
	OMS-708
Inchi:	InChI=1S/C10H9NO2S/c1-11-10(12)13-8-3-2-4-9-7(8)5-6-14-9/h2-6H,1H3,(H,11,12)
InchiKey:	BOTUVXISJHKZKJ-UHFFFAOYSA-N
Formula:	C10H9NO2S
SMILES:	CNC(=O)Oc1cccc2sccc12
Mol. weight [g/mol]:	207.25
CAS:	1079-33-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	2.619		Crippen Method
mcvol	146.610	ml/mol	McGowan Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tf	402.80 ± 0.20	K	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=C1079330&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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point