2,4-dimethyl-3-oxa-8-thiabicyclo[3.3.0]-1,4-octadie

Inchi: InChI=1S/C8H10OS/c1-5-7-3-4-10-8(7)6(2)9-5/h3-4H2,1-2H3
InchiKey: BZLYSXAGISNIGC-UHFFFAOYSA-N
Formula: C8H10OS
SMILES: Cc1oc(C)c2c1CCS2
Mol. weight [g/mol]: 154.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.18		Crippen Method
logp	2.545		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
ripol	1779.00		NIST Webbook
ripol	1779.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R489746&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.