S-triazolo(2,3-a)pyrimidin-7-ol, 2-trifluoromethyl-5-methyl-

Inchi: InChI=1S/C7H5F3N4O/c1-3-2-4(15)14-6(11-3)12-5(13-14)7(8,9)10/h2,15H,1H3
InchiKey: ABRJUSGRGBUWOM-UHFFFAOYSA-N
Formula: C7H5F3N4O
SMILES: Cc1cc(O)n2nc(C(F)(F)F)nc2n1
Mol. weight [g/mol]: 218.14
CAS: 116529-17-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Crippen Method
logp	1.157		Crippen Method
mcvol	121.670	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C116529170&Units=SI

Legend

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