4H-3,1-benzoxazine-4-one, 2-trifluoromethyl-

Inchi: InChI=1S/C9H4F3NO2/c10-9(11,12)8-13-6-4-2-1-3-5(6)7(14)15-8/h1-4H
InchiKey: GHLXPUXNDMOETG-UHFFFAOYSA-N
Formula: C9H4F3NO2
SMILES: O=c1oc(C(F)(F)F)nc2ccccc12
Mol. weight [g/mol]: 215.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	2.207		Crippen Method
mcvol	121.480	ml/mol	McGowan Method
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375136&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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