5-Acetamino-1-[2,6-dichloro-4-(trifluoromethyl)ph

Inchi: InChI=1S/C14H6Cl2F6N4O2S/c1-5(27)24-12-11(29(28)14(20,21)22)9(4-23)25-26(12)10-
InchiKey: BICHUEJEIVUZMZ-UHFFFAOYSA-N
Formula: C14H6Cl2F6N4O2S
SMILES: CC(=O)Nc1c(S(=O)C(F)(F)F)c(C#N)nn1-c1c(Cl)cc(C(F)(F)F)cc1Cl
Mol. weight [g/mol]: 479.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.57		Crippen Method
logp	4.655		Crippen Method
mcvol	255.110	ml/mol	McGowan Method
rinpol	1968.00		NIST Webbook

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=U372985&Units=SI

Legend

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