



Dataset Name  
 Entry Label  
 Canonical SMILES  
 Torsion Atom Indices  
 Torsion SMIRKS  
 Torsion SMIRKS ID  
 SMIRKS Total Count

OpenFF Group1 Torsions  
C[C:2](=[0:1])[N:3](C)[c:4]1[nH]ccn1  
CC(=O)N(C)c1[nH]ccn1  
 [9, 3, 8, 2]  
[\*:1]-[#7X3:2]-!@[#6X3:3](=[#8,#16,#7:4])-[#6,#1]  
 t70b  
 1