

properties

fragmentsWithSugar  
fragments  
xRefs  
foundInDatabases  
bcutDescriptor  
ertlFunctionalFragments  
ertlFunctionalFragmentsPseudoSmiles  
absoluteSmilesSources  
synonyms  
citationDoi  
geoLocation  
textTaxa  
containsSugar  
fragmentComplexityDescriptor  
bondCount  
idInSource  
isTopological  
heavyAtomNumber  
fmfDescriptor  
eccentricConnectivityIndexDescriptor  
maxNumberOfRings  
petitjeanNumber  
nameTrustLevel  
cleanSmiles  
annotationLevel  
sugarFreeSmiles  
aquisitionDate  
source  
bpol  
sugarFreeTotalAtomNumber  
kappaShapeIndex2  
molecularWeight  
isElectronic  
wienerPathNumber  
totalAtomNumber  
zagrebIndex  
isMolecular  
simpleInchi  
vabcDescriptor  
gravitationalIndexHeavyAtoms  
manholdlogp  
kappaShapeIndex1  
xlogp  
apol  
circularFingerprint  
uniqueSmiles  
numberSpiroAtoms  
molecularFormula  
numberOfNitrogens  
vertexAdjMagnitude  
hBondAcceptorCount  
numberOfOxygens  
containsLinearSugars  
lipinskiRuleOf5Failures  
hBondDonorCount  
pubchemFingerprint  
minNumberOfRings  
containsRingSugars  
sugarFreeHeavyAtomNumber  
simpleSmiles  
petitjeanShapeGeom  
fsp3  
wienerPolarityNumber  
numberOfCarbons  
dataOriginatedFrom  
simpleInchiKey  
petitjeanShapeTopo  
isIdentifiedBy  
smiles  
pubchemBits  
isGeometrical  
isConstitutional  
kappaShapeIndex3  
extendedFingerprint  
pubchemBitsString  
hybridizationRatioDescriptor  
tpsaEfficiency  
alogp  
amralogp  
topoPSA  
alogp2  
originalSmiles  
nplSugarScore  
nplNohScore  
nplScore  
murkoFramework  
cas  
name  
originalInchi  
originalInchiKey  
taxonomyReferenceObjects

