

property

xRefs
foundInDatabases
bcutDescriptor
absoluteSmilesSources
synonyms
citationDoi
geoLocation
textTaxa
simpleInchiKey
hasMolecularDescriptors
idInSource
dataOriginatedFrom
hBondDonorCount
bpol
fragmentComplexityDescriptor
hasMolecularFeatures
numberOfCarbons
minNumberOfRings
aquisitionDate
heavyAtomNumber
fmfDescriptor
cleanSmiles
kappaShapeIndex2
molecularWeight
vertexAdjMagnitude
wienerPolarityNumber
hasGeolocation
containsLinearSugars
petitjeanNumber
hasTaxonomyData
circularFingerprint
fsp3
source
uniqueSmiles
zagrebIndex
simpleSmiles
sugarFreeTotalAtomNumber
xlogp
vabcDescriptor
hasMolecularProperties
manholdlogp
numberOfNitrogens
simpleInchi
containsRingSugars
petitjeanShapeGeom
extendedFingerprint
hasAnalyticData
hasCitation
maxNumberOfRings
totalAtomNumber
bondCount
containsSugar
wienerPathNumber
numberSpiroAtoms
apol
kappaShapeIndex1
pubchemBits
sugarFreeHeavyAtomNumber
numberOfOxygens
hBondAcceptorCount
petitjeanShapeTopo
eccentricConnectivityIndexDescriptor
hasFingerprint
kappaShapeIndex3
lipinskiRuleOf5Failures
gravitationalIndexHeavyAtoms
molecularFormula
sugarFreeSmiles
smiles
isIdentifiedBy
pubchemFingerprint
hybridizationRatioDescriptor
topoPSA
alogp
alogp2
amralogp
tpsaEfficiency
originalSmiles
nplNohScore
nplScore
nplSugarScore
murkoFramework
name
originalInchi
originalInchiKey
taxonomyReferenceObjects

