

Name	Description
fr_NH0	Number of Tertiary amines
RingCount	Number of Ring
PEOE_VSA9	Hybrid descriptors derived from van der Waals surface area and atomic Gasteiger partial charges
fr_Ar_N	Number of aromatic nitrogens
MaxAbsEStateIndex	Maximum absolute value of electrotopological state indices for all atoms
SlogP_VSA5	Hybrid descriptors derived from van der Waals surface area and logP(o/w)
BertzCT	Topological index used to quantify the complexity of the bonding and complexity of the distribution of heteroatoms
NumAromaticRings	Number of aromatic rings
NumSaturatedHeterocycles	Number of saturated heterocycles
SlogP_VSA6	Hybrid descriptors derived from van der Waals surface area and logP(o/w)
fr_Ar_NH	Number of aromatic amines
NumAliphaticHeterocycles	Number of aliphatic (containing at least one non-aromatic bond) heterocycles
HallKierAlpha	the topological state and a topological index by Hall and Kier
fr_unbrch_alkane	Number of unbranched alkanes of at least 4 members (excludes halogenated alkanes)
fr_benzene	Number of benzene rings
FractionCSP3	Number of the fraction of C atoms that are SP3 hybridized
SlogP_VSA10	Hybrid descriptors derived from van der Waals surface area and logP(o/w)
qed	the weighted sum of ADS mapped properties
fr_Al_COO	Number of aliphatic carboxylic acids
fr_urea	Number of urea groups
SMR_VSA3	Hybrid descriptors derived from van der Waals surface area calculated and molecular refractivity properties
SMR_VSA5	Hybrid descriptors derived from van der Waals surface area calculated and molecular refractivity properties
EState_VSA11	Hybrid descriptors derived from van der Waals surface area and electrotopological state indices
fr_aniline	Number of anilines
fr_Al_OH_noTert	Number of aliphatic hydroxyl groups excluding tert-OH
NumAromaticHeterocycles	Number of aromatic heterocycles
Chi4v	Molecular connectivity Chi indexes
SlogP_VSA2	Hybrid descriptors derived from van der Waals surface area and logP(o/w)
Chi4n	Molecular connectivity Chi indexes

Chi1	Molecular connectivity Chi indexes
SlogP_VSA8	Hybrid descriptors derived from van der Waals surface area and logP(o/w)
MinPartialCharge	Minimum amount of charge for a molecule
NumHAcceptors	Number of Hydrogen Bond Acceptors
PEOE_VSA3	Hybrid descriptors derived from van der Waals surface area and atomic Gasteiger partial charges
fr_ArN	Number of N functional groups attached to aromatics
PEOE_VSA11	Hybrid descriptors derived from van der Waals surface area and atomic Gasteiger partial charges
SMR_VSA4	Hybrid descriptors derived from van der Waals surface area calculated and molecular refractivity properties
NumHeteroatoms	Number of heteroatoms
EState_VSA7	Hybrid descriptors derived from van der Waals surface area and electrotopological state indices
fr_allylic_oxid	Number of allylic oxidation sites excluding steroid dienone
NumSaturatedRings	Number of saturated rings
fr_lactone	Number of cyclic esters (lactones)
fr_N_O	Number of hydroxylamine groups
NumSaturatedCarbocycles	Number of saturated carbocycles
NumAliphaticCarbocycles	Number of aliphatic (containing at least one non-aromatic bond) carbocycles
fr_priamide	Number of primary amides
fr_thiazole	Number of thiazole rings
PEOE_VSA8	Hybrid descriptors derived from van der Waals surface area and atomic Gasteiger partial charges
SMR_VSA10	Hybrid descriptors derived from van der Waals surface area calculated and molecular refractivity properties
Chi2v	Molecular connectivity Chi indexes
EState_VSA4	Hybrid descriptors derived from van der Waals surface area and electrotopological state indices
PEOE_VSA12	Hybrid descriptors derived from van der Waals surface area and atomic Gasteiger partial charges
SlogP_VSA4	Hybrid descriptors derived from van der Waals surface area and logP(o/w)
fr_Ar_OH	Number of aromatic hydroxyl groups
PEOE_VSA10	Hybrid descriptors derived from van der Waals surface area and atomic Gasteiger partial charges
fr_ester	Number of esters
PEOE_VSA1	Hybrid descriptors derived from van der Waals surface area and atomic Gasteiger partial charges
TPSA	Polar surface area
PEOE_VSA7	Hybrid descriptors derived from van der Waals surface area and atomic Gasteiger partial charges

Kappa3	Molecular connectivity Kappa indexes
NumAliphaticRings	Number of aliphatic (containing at least one non-aromatic bond) rings
fr_pyridine	Number of pyridine rings
SlogP_VSA3	Hybrid descriptors derived from van der Waals surface area and logP(o/w)
EState_VSA2	Hybrid descriptors derived from van der Waals surface area and electrotopological state indices
NHOHCount	Number of NHs or OHs
MinAbsPartialCharge	Maximum absolute value of charge
SMR_VSA6	Hybrid descriptors derived from van der Waals surface area calculated and molecular refractivity properties
fr_imidazole	Number of imidazole rings
fr_amide	Number of amides
