

Descriptor	Complete dataset	Refined dataset	Name	Description
ATSC8e	1	0	2D autocorrelations	Centred Broto-Moreau autocorrelation of lag 8 weighted by Sanderson electronegativity
ATSC3e	1	0	2D autocorrelations	Centred Broto-Moreau autocorrelation of lag 3 weighted by Sanderson electronegativity
P_VSA_s_6	1	0	P_VSA-like descriptors	P_VSA-like on I-state, bin 6
SM1_B(s)	1	0	2D matrix-based descriptors	spectral moment of order 1 from Burden matrix weighted by I-State
SM1_Dz(m)	1	0	2D matrix-based descriptors	spectral moment of order 1 from Barysz matrix weighted by mass
MATS2m	1	1	2D autocorrelations	Moran autocorrelation of lag 2 weighted by mass
ATSC2s	1	0	2D autocorrelations	Centred Broto-Moreau autocorrelation of lag 2 weighted by I-state
SM1_Dz(v)	1	0	2D matrix-based descriptors	spectral moment of order 1 from Barysz matrix weighted by van der Waals volume
SAacc	1	0	Molecular properties	surface area of acceptor atoms from P_VSA-like descriptors
P_VSA_p_2	1	0	P_VSA-like descriptors	P_VSA-like on polarizability, bin 2
P_VSA_m_3	1	0	P_VSA-like descriptors	P_VSA-like on mass, bin 3
ATSC3s	1	0	2D autocorrelations	Centred Broto-Moreau autocorrelation of lag 3 weighted by I-state
ATSC1s	1	0	2D autocorrelations	Centred Broto-Moreau autocorrelation of lag 1 weighted by I-state
IC1	1	1	Information indices	Information Content index (neighborhood symmetry of 1-order)
P_VSA_v_2	1	0	P_VSA-like descriptors	P_VSA-like on van der Waals volume, bin 2
CATS2D_09_DL	1	1	CATS 2D	CATS2D Donor-Lipophilic at lag 09
TPSA(NO)	1	1	Molecular properties	topological polar surface area using N,O polar contributions
TPSA(Tot)	1	1	Molecular properties	topological polar surface area using N,O,S,P polar contributions
P_VSA_LogP_4	1	1	P_VSA-like descriptors	P_VSA-like on LogP, bin 4
ATSC1e	1	1	2D autocorrelations	Centred Broto-Moreau autocorrelation of lag 1 weighted by Sanderson electronegativity
SpPosA_B(m)	0	1	2D matrix-based descriptors	normalized spectral positive sum from Burden matrix weighted by mass
SpPosA_B(e)	0	1	2D matrix-based descriptors	normalized spectral positive sum from Burden matrix weighted by Sanderson electronegativity
AMW	0	1	Constitutional indices	average molecular weight

AAC	0	1	Information indices	mean information index on atomic composition
SpPosA_B(i)	0	1	2D matrix-based descriptors	normalized spectral positive sum from Burden matrix weighted by ionization potential
SIC3	0	1	Information indices	Structural Information Content index (neighborhood symmetry of 3-order)
SIC1	0	1	Information indices	Structural Information Content index (neighborhood symmetry of 1-order)
IC0	0	1	Information indices	Information Content index (neighborhood symmetry of 0-order)
H%	0	1	Constitutional indices	percentage of H atoms
CIC1	0	1	Information indices	Complementary Information Content index (neighborhood symmetry of 1-order)
ChiA_B(s)	0	1	2D matrix-based descriptors	average Randic-like index from Burden matrix weighted by I-State
Me	0	1	Constitutional indices	mean atomic Sanderson electronegativity (scaled on Carbon atom)
SM1_Dz(Z)	0	1	2D matrix-based descriptors	spectral moment of order 1 from Barysz matrix weighted by atomic number

1: presence

0: absence