

Sample 599 SHAP Waterfall Plot

 $f(x) = 12.63$

MolLogP

+4.47

TPSA

-1.15

NumAromaticRings

-0.94

NumHAcceptors

+0.55

NumHDonors

-0.53

NumRotatableBonds

-0.14

LabuteASA

-0.14

MolWt

+0.08

NumSaturatedRings

+0.05

NumAliphaticRings

-0.03

9

10

11

12

 $E[f(X)] = 10.417$ 