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Q SAR

System: Class: Reference:

Action: Compound: Year:

Parameters: Substituents: SMILES:

Equation Terms: N: SD: R²:

Stars: Listing Type: Sort Type: Set No:

Set	N	SD	R ²	Q ²	Stars	Opt	Action	Equation
3811	23	0.576	0.852	0.761	★★★★★			$\log \frac{1}{C} = 1.7 \cdot \text{ClogP} - 1.0 \cdot \text{I,COOH} - 1.4 \cdot \text{I-CF}_3 - 1.2 \cdot \sigma^+, \text{R}_1 + 1.2$
10772	15	0.308	0.902	0.801	★★★★☆	3.261		$\log \frac{1}{C} = 7.5 \cdot \text{ClogP} - 1.1 \cdot \text{ClogP}^2 + 1.2 \cdot \text{I,X} - 7.4$
11034	6	0.528	0.876	0.677	★★★★☆			$\log \frac{1}{C} = -2.8 \cdot \text{MgVol} + 10.7$

Set	3811
System	HUMAN CYCLOOXYGENASE-2 ENZYME
Class	Oxidoreductases
Compound	3-R2-5-(R1-C6H4)-1-(C6H4-4-SO2NH2)-PYRAZOLES
Action	IC ₅₀ ENZYME INHIBITION
Reference	PENNING, T.D., TALLEY, J.J., BERTENSHAW, S.R., CARTER, J.S., COLLINS, P.W., DOCTER, S., GRANETO, M.J., LEE, L.F., MALECHA, J.W., MIYASHIRO, J.M., ROGERS, R.S., ROGIER, D.J., YU, S.S., ANDERSON, G.D., BURTON, E.G., COGBURN, J.N., GREGORY, S.A., KOBOLDT, C.M., PERKINS, W.E., SEIBERT, K., VEENHUIZEN, A.W., ZHANG, Y.Y., ISAKSON, P.C. J.MED.CHEM. 40, 1347-1365 (1997) R3669
Note	I,COOH = 1.0 FOR COOH GROUP OF R1
Parameters	$\log \frac{1}{C} \sigma, \text{R}_1 \sigma^+, \text{R}_1 \sigma^-, \text{R}_1 \text{B5-R1,2 B5-R1,3 B5-R1,4 I,COOH } \pi\text{-R1,4 I-CF}_3 \text{ ClogP CMR MgVol BILIN(ClogP)}$

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The Toolbox is a free software application that supportsreproducible and transparent chemical hazard assessment.

Set N SD R² Q² Stars Opt Action Equation

Set	N	SD	R²	Q²	Stars	Opt	Action	Equation
3811	23	0.576	0.852	0.761	★★★★★			$\log \frac{1}{C} = 1.7 \cdot \text{ClogP} - 1.0 \cdot I, \text{COOH} - 1.4 \cdot I\text{-CF}_3 - 1.2 \cdot \sigma^+, R_1 + 1.2$
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Note	I, COOH = 1.0 FOR COOH GROUP OF R1
Parameters	$\log \frac{1}{C}$, σ , R1, σ^+ , R1, B5-R1,2, B5-R1,3, B5-R1,4, I, COOH, π -R1,4, I-CF3, ClogP, CMR, MgVol, BILIN(ClogP)

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