



Formula: C<sub>31</sub>H<sub>48</sub>O<sub>2</sub>S<sub>2</sub>

MW: 516.85

CAS: 23288-49-5

MDL NUMBER: MFCD00079281

IUPAC: 2,6-bis(tert-butyl)-4-{1-[3,5-bis(tert-butyl)-4-hydroxyphenylthio]-isopropylthio}phenol

Smiles: c1(c(C(C)(C)C)cc(SC(Sc2cc(C(C)(C)C)c(c(c2)C(C)(C)C)O)(C)C)cc1C(C)(C)C)O

THERAPEUTIC CATEGORY: Antihyperlipoproteinemic

REFERENCE: Merck 13, 7844 Barnhart JW, et al. Hypocholesterolemic effect of 4,4'-(isopropylidenedithio)-bis(2,6-di-t-butylphenol) (probucol). Am J Clin Nutr. 1970 Sep;23(9):1229-33

ACCEPTORS: 2

DONORS: 2

ROTATION BONDS: 4

N+O: 2

Chiral Centers: 0

LogP: 13.24

LogS: -8.51

LIPINSKI: 2

Synonyms: PROBUCOL;4,4