

Estimation of Physical-Chemical Property and Environmental Fate of
Benzoyl peroxide Using (Q)SAR

Mi Kyoung Kim, Su-Hyon Kim, Heekyung Bae, Sanghwan Song, Hyunju
Koo, Moon-Soon Lee, Seong-Hwan Jeon, Jin-Gyun Na and Kwangsik
Park¹

*National Institute of Environmental Research, Gyeongseo-dong,
Seo-gu, Incheon 404-170, Korea*

¹*College of Pharmacy, Dongduk Women's University 23-1, Wolgok-dong,
Seongbuk-gu, Seoul 136-174, Korea*

Abstract

Benzoyl peroxide is a High Production Volume Chemical, which is produced about 1,375 tons/year in Korea as of 2001 survey. The substance is mainly used as initiators in polymerization, catalysts in the plastics industry, bleaching agents for flour and medication for acne vulgaris. The substance is one of seven chemicals of which human health and environmental risks are being assessed by National Institute of Environmental Research (NIER) under the frame of OECD SIDS Program. In this study, Quantitative Structure-Activity Relationships (QSAR) is used for getting adequate information on the physical-chemical property and the environmental fate of this chemical. For the assessment of benzoyl peroxide, models such as MPBPWIN for vapor pressure, KOWWIN for octanol/water partition coefficient, HENRYWIN for Henry's Law constant, AOPWIN for photolysis and BCFWN for bioconcentration factor (BCF) were used. These (Q)SAR model programmes were worked by using the SMILES (Simplified Molecular Input Line Entry System) notations. The physical-chemical properties and the environmental fate of benzoyl peroxide were estimated as followed : vapor pressure = 0.00929 Pa, Log Kow = 3.43, Henry's Law constant = 0.00000354 atm-m³/mole at 25 °C, the half-life of photodegradation = 3 days, bioconcentration factor (BCF) = 92

<책임연구자>

성 명 : 이 문 순

주 소 : 인천광역시 서구 경서동 종합환경연구단지 국립환경연구원

연락처 : 전화(032-560-7113), 팩스(032-568-2037), E-mail(mslee416@me.go.kr)