

## Accepted Manuscript

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PII: S0021-9614(18)30536-6  
DOI: <https://doi.org/10.1016/j.jct.2018.09.006>  
Reference: YJCHT 5535

To appear in: *J. Chem. Thermodynamics*

Received Date: 22 May 2018  
Revised Date: 11 September 2018  
Accepted Date: 12 September 2018

Please cite this article as: X. Liu, X. Zhang, Solvent screening and liquid-liquid measurement for extraction of phenols from aromatic hydrocarbon mixtures, *J. Chem. Thermodynamics* (2018), doi: <https://doi.org/10.1016/j.jct.2018.09.006>

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# Solvent screening and liquid-liquid measurement for extraction of phenols from aromatic hydrocarbon mixtures

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**ABSTRACT:** The separation of phenolic compounds from low temperature coal tar has great significance for further application of the coal tar. In this paper, the separation of special phenolic compounds from model coal tar (phenols + toluene) was studied. The universal quasi chemical functional group activity coefficient (UNIFAC) and conductor-like screening model COSMO-SAC (segment activity coefficient) was carried out to screen suitable solvent. Ethylene glycol was selected as the potential solvent to extract the phenols from aromatic hydrocarbon, evaluated by area of two-phase region and the criterion of solvent power ( $SP_i^\infty$ ), selectivity ( $S^\infty$ ) and performance index (PI). Liquid-liquid equilibria of the ethylene glycol + phenols + toluene ternary systems were measured in the temperature range (303.15-323.15) K under 101.3 kPa, and the results showed that ethylene glycol has a high extraction efficiency with distribution coefficient (between 2 and 12) and selectivity (between 7 and 255). Moreover, the NRTL and UNIQUAC models were successfully applied to correlate the experimental LLE data with RMSD less than 1.85%, indicating that both models can accurately describe LLE behaviour of this system. Thus, the corresponding binary interaction parameters would be helpful for separation process designing or optimizing.

**Keywords:** Liquid-liquid equilibria; toluene; ethylene glycol; phenols; COSMO-SAC.

## 1. Introduction

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