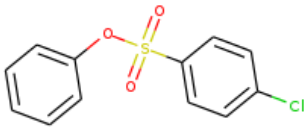
Phenyl p-chloro-benzene sulfonate

InChI: InChI=1S/C12H9ClO3S/c13-10-6-8-12(9-7-10)17(14,15)16-11-4-2-1-3-5-11/h1-9H
InChI Key: FQIJSBUGQPNMQA-UHFFFAOYSA-N
Formula: C12H9ClO3S
SMILES: O=S(=O)(Oc1ccccc1)c1ccc(Cl)cc1
Molecular Weight: 268.72
CAS: 2437-33-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-320.12	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-430.73	kJ/mol	Joback Method
$\Delta_{fus} H°$	31.29	kJ/mol	Joback Method
$\Delta_{vap} H°$	72.95	kJ/mol	Joback Method
$logP_{oct/wat}$	3.11		Crippen Method
P_c	3801.00	kPa	Joback Method
T_{boil}	639.93	K	Joback Method
T_c	879.02	K	Joback Method
T_{fus}	381.07	K	Joback Method
V_c	0.68	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	409.44	J/mol×K	639.93	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H9ClO3S/c13-10-6-8-12(9-7-10)17(14,15)16-11-4-2-1-3-5-11/h1-9H

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).