3-Bromobenzoic acid, 2-chlorophenyl ester

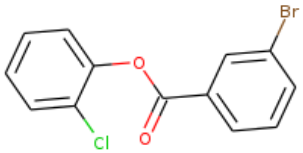
InChI: InChI=1S/C13H8BrClO2/c14-10-5-3-4-9(8-10)13(16)17-12-7-2-1-6-11(12)15/h1-8H

InChI Key: GLMMOSUCBIPMQS-UHFFFAOYSA-N

Formula: C13H8BrClO2

SMILES: O=C(Oc1ccccc1Cl)c1cccc(Br)c1

Molecular Weight: 311.56



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	32.61	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-95.74	kJ/mol	Joback Method
$\Delta_{fus} H°$	29.00	kJ/mol	Joback Method
$\Delta_{vap} H°$	70.38	kJ/mol	Joback Method
$logP_{oct/wat}$	4.322		Crippen Method
P_c	3243.03	kPa	Joback Method
T_{boil}	740.04	K	Joback Method
T_c	1003.05	K	Joback Method
T_{fus}	476.03	K	Joback Method
V_c	0.682	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	419.51	J/mol×K	740.04	Joback Method
η	0.0001388	Pa×s	740.04	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H8BrClO2/c14-10-5-3-4-9(8-10)13(16)17-12-7-2-1-6-11(12)15/h1-8H
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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