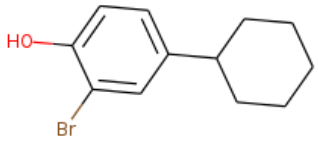
2-Bromo-4-cyclohexyl-phenol

InChI: InChI=1S/C12H15BrO/c13-11-8-10(6-7-12(11)14)9-4-2-1-3-5-9/h6-9,14H,1-5H2
InChI Key: DSYPBKQKCSJRHB-UHFFFAOYSA-N
Formula: C12H15BrO
SMILES: Oc1ccc(C2CCCCC2)cc1Br
Molecular Weight: 255.15
CAS: 15460-06-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	37.09	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-162.61	kJ/mol	Joback Method
$\Delta_{fus} H°$	23.39	kJ/mol	Joback Method
$\Delta_{vap} H°$	65.12	kJ/mol	Joback Method
$logP_{oct/wat}$	4.20		Crippen Method
P_c	3759.17	kPa	Joback Method
T_{boil}	671.95	K	Joback Method
T_c	936.82	K	Joback Method
T_{fus}	442.84	K	Joback Method
V_c	0.56	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	434.58	J/mol×K	671.95	Joback Method
η	0.00	Pa×s	671.95	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H15BrO/c13-11-8-10(6-7-12(11)14)9-4-2-1-3-5-9/h6-9,14H,1-5H2
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).