Benzoic acid, 3-bromo-, methyl ester

Other names: 3-Bromobenzoic acid, methyl ester; Benzoic acid, m-bromo-, methyl ester; Methyl 3-bromobenzoate; Methyl m-bromobenzoate; m-Bromobenzoic acid methyl ester.

InChI: InChI=1S/C8H7BrO2/c1-11-8(10)6-3-2-4-7(9)5-6/h2-5H,1H3

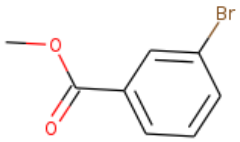
InChI Key: KMFJVYMFCAIRAN-UHFFFAOYSA-N

Formula: C8H7BrO2

SMILES: COC(=O)c1cccc(Br)c1

Molecular Weight: 215.04

CAS: 618-89-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-100.34	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-201.86	kJ/mol	Joback Method
$\Delta_{fus} H°$	18.20	kJ/mol	Joback Method
$\Delta_{vap} H°$	51.93	kJ/mol	Joback Method
$logP_{oct/wat}$	2.24		Crippen Method
P_c	4135.61	kPa	Joback Method
T_{boil}	395.70	K	NIST Webbook
T_{boil}	395.60	K	NIST Webbook
T_c	792.86	K	Joback Method
T_{fus}	304.50 ± 0.50	K	NIST Webbook
V_c	0.46	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	246.83	J/mol×K	556.55	Joback Method
η	0.00	Pa×s	556.55	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H7BrO2/c1-11-8(10)6-3-2-4-7(9)5-6/h2-5H,1H3
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).