2-Propenoic acid, 3-(4-bromophenyl)-, ethyl ester

Other names: 2-Propenoic acid, 3-(4-bromophenyl)-, ethyl ester; Cinnamic acid, p-bromo-, ethyl ester, (E)-; Ethyl (2E)-3-(4-bromophenyl)-2-propenoate; Ethyl trans-4-bromocinnamate; trans-p-Bromocinnamic acid ethyl ester.

InChI: InChI=1S/C11H11BrO2/c1-2-14-11(13)8-5-9-3-6-10(12)7-4-9/h3-8H,2H2,1H3/b8-5+

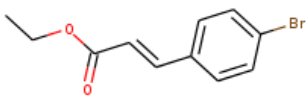
InChI Key: YOOKYIPLSLPRTC-VMPITWQZSA-N

Formula: C11H11BrO2

SMILES: CCOC(=O)C=Cc1ccc(Br)cc1

Molecular Weight: 255.11

CAS: 24393-53-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	5.14	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-146.56	kJ/mol	Joback Method
$\Delta_{fus} H°$	26.17	kJ/mol	Joback Method
$\Delta_{vap} H°$	58.57	kJ/mol	Joback Method
$log P_{oct/wat}$	3.025		Crippen Method
P_c	3117.52	kPa	Joback Method
T_{boil}	453.20	K	NIST Webbook
T_c	861.83	K	Joback Method
T_{fus}	379.55	K	Joback Method
V_c	0.610	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	363.25	J/mol×K	629.35	Joback Method
η	0.0001643	Pa×s	629.35	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H11BrO2/c1-2-14-11(13)8-5-9-3-6-10(12)7-4-9/h3-8H,2H2,1H3/b8-5+

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).