

3-Bromobenzoic acid. 3-methylbut-2-enyl ester

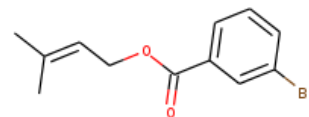
InChI: InChI=1S/C12H13BrO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-6,8H,7H2,1-2H3

InChI Key: SCHFXORPCOMCOF-UHFFFAOYSA-N

Formula: C12H13BrO2

SMILES: CC(C)=CCOC(=O)c1cccc(Br)c1

Molecular Weight: 269.13



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	5.01	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-176.99	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	27.45	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	60.87	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.57		Crippen Method
P_c	2823.32	kPa	Joback Method
T_{boil}	652.11	K	Joback Method
T_c	884.01	K	Joback Method
T_{fus}	376.86	K	Joback Method
V_c	0.67	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	411.62	J/mol×K	652.11	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H13BrO2/c1-9\(2\)6-7-15-12\(14\)10-4-3-5-11\(13\)8-10/h3-6,8H,7H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H13BrO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-6,8H,7H2,1-2H3)

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

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: 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 (m³/kg-mol).

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