

3-Bromobenzoic acid, oct-3-en-2-yl ester

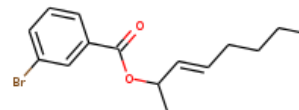
InChI: InChI=1S/C15H19BrO2/c1-3-4-5-6-8-12(2)18-15(17)13-9-7-10-14(16)11-13/h6-12H,3-5H2,1-2H3/b8-6+

InChI Key: UOEBIVUSZSTAHC-SOFGYWHQSA-N

Formula: C15H19BrO2

SMILES: CCCCC=CC(C)OC(=O)c1cccc(Br)c1

Molecular Weight: 311.21



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	36.38	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-234.40	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	33.01	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	67.08	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.74		Crippen Method
P_c	2129.52	kPa	Joback Method
T_{boil}	720.43	K	Joback Method
T_c	940.78	K	Joback Method
T_{fus}	409.63	K	Joback Method
V_c	0.83	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	566.72	J/mol×K	720.43	Joback Method
η	0.00	Paxs	720.43	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H19BrO2/c1-3-4-5-6-8-12\(2\)18-15\(17\)13-9-7-10-14\(16\)11-13/h6-12H,3-5H2,1-2H3/b8-6+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H19BrO2/c1-3-4-5-6-8-12(2)18-15(17)13-9-7-10-14(16)11-13/h6-12H,3-5H2,1-2H3/b8-6+)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, \text{gas}}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

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

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

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

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

$\log P_{\text{oct/wat}}$: 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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