

2-Bromobenzyl alcohol, 2-methylbutyl ether

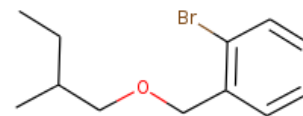
InChI: InChI=1S/C12H17BrO/c1-3-10(2)8-14-9-11-6-4-5-7-12(11)13/h4-7,10H,3,8-9H2,1-2H3

InChI Key: PBDRFSROPYAYMA-UHFFFAOYSA-N

Formula: C12H17BrO

SMILES: CCC(C)COCc1ccccc1Br

Molecular Weight: 257.17



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	59.82	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-177.12	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	23.44	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	53.70	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.012		Crippen Method
P_c	2515.07	kPa	Joback Method
T_{boil}	593.76	K	Joback Method
T_c	810.17	K	Joback Method
T_{fus}	330.97	K	Joback Method
V_c	0.673	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	416.98	J/mol×K	593.76	Joback Method
η	0.0001556	Paxs	593.76	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H17BrO/c1-3-10\(2\)8-14-9-11-6-4-5-7-12\(11\)13/h4-7,10H,3,8-9H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H17BrO/c1-3-10(2)8-14-9-11-6-4-5-7-12(11)13/h4-7,10H,3,8-9H2,1-2H3)

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

Legend

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

η : Dynamic viscosity (Pa \times s).

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

$\Delta_f H^\circ_{gas}$: 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).

$logP_{oct/wat}$: 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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