2-Bromobenzyl alcohol, 2-methylbutyl ether

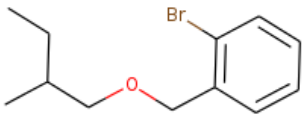
InChI: InChI=1S/C12H17BrO/c1-3-10(2)8-14-9-11-6-4-5-7-12(11)13/h4-7,10H,3,8-9H2,1-2H3

InChI Key: PBDRFSROPYAYMA-UHFFFAOYSA-N

Formula: C12H17BrO

SMILES: CCC(C)COCc1ccccc1Br

Molecular Weight: 257.17



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	59.82	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-177.12	kJ/mol	Joback Method
$\Delta_{fus} H°$	23.44	kJ/mol	Joback Method
$\Delta_{vap} H°$	53.70	kJ/mol	Joback Method
$logP_{oct/wat}$	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
$C_{p,gas}$	416.98	J/mol×K	593.76	Joback Method
η	0.0001556	Pa×s	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
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).