

2-Bromobenzyl alcohol, 2-methylpropyl ether

Inchi:	InChI=1S/C11H15BrO/c1-9(2)7-13-8-10-5-3-4-6-11(10)12/h3-6,9H,7-8H2,1-2H3
InchiKey:	SDHOXPABQZEJNM-UHFFFAOYSA-N
Formula:	C11H15BrO
SMILES:	CC(C)COCc1ccccc1Br
Mol. weight [g/mol]:	243.14

Physical Properties

Property code	Value	Unit	Source
gf	51.40	kJ/mol	Joback Method
hf	-156.48	kJ/mol	Joback Method
hfus	20.85	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.622		Crippen Method
mcvol	165.460	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1476.00		NIST Webbook
tb	570.88	K	Joback Method
tc	791.16	K	Joback Method
tf	319.70	K	Joback Method
vc	0.618	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.86	J/molxK	570.88	Joback Method
cpg	383.64	J/molxK	607.59	Joback Method
cpg	397.55	J/molxK	644.31	Joback Method
cpg	410.62	J/molxK	681.02	Joback Method
cpg	422.89	J/molxK	717.73	Joback Method
cpg	434.38	J/molxK	754.45	Joback Method
cpg	445.12	J/molxK	791.16	Joback Method
dvisc	0.0019905	Paxs	319.70	Joback Method
dvisc	0.0010473	Paxs	361.56	Joback Method

dvisc	0.0006296	Paxs	403.43	Joback Method
dvisc	0.0004165	Paxs	445.29	Joback Method
dvisc	0.0002958	Paxs	487.15	Joback Method
dvisc	0.0002218	Paxs	529.02	Joback Method
dvisc	0.0001735	Paxs	570.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378180&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/49-373-4/2-Bromobenzyl-alcohol-2-methylpropyl-ether.pdf>

Generated by Cheméo on 2024-04-19 15:38:15.116191578 +0000 UTC m=+15830344.036768890.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.