

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
InchiKey:	PBDRFSROPYAYMA-UHFFFAOYSA-N
Formula:	C12H17BrO
SMILES:	CCC(C)COCc1ccccc1Br
Mol. weight [g/mol]:	257.17

Physical Properties

Property code	Value	Unit	Source
gf	59.82	kJ/mol	Joback Method
hf	-177.12	kJ/mol	Joback Method
hfus	23.44	kJ/mol	Joback Method
hvap	53.70	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.012		Crippen Method
mcvol	179.550	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinqol	1584.00		NIST Webbook
tb	593.76	K	Joback Method
tc	810.17	K	Joback Method
tf	330.97	K	Joback Method
vc	0.673	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.98	J/molxK	593.76	Joback Method
cpg	432.48	J/molxK	629.83	Joback Method
cpg	447.08	J/molxK	665.90	Joback Method
cpg	460.81	J/molxK	701.97	Joback Method
cpg	473.69	J/molxK	738.04	Joback Method
cpg	485.77	J/molxK	774.10	Joback Method
cpg	497.07	J/molxK	810.17	Joback Method
dvisc	0.0018986	Paxs	330.97	Joback Method
dvisc	0.0009820	Paxs	374.77	Joback Method

dvisc	0.0005830	Paxs	418.57	Joback Method
dvisc	0.0003821	Paxs	462.37	Joback Method
dvisc	0.0002694	Paxs	506.16	Joback Method
dvisc	0.0002008	Paxs	549.96	Joback Method
dvisc	0.0001563	Paxs	593.76	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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