

Benzhydrol, 4-bromo-

Other names:	p-Bromobenzhydrol 4-Bromobenzhydrol Benzenemethanol, 4-bromo-«alpha»-phenyl- (4-Bromophenyl)phenylmethanol Phenyl-p-bromophenyl methanol p-bromobenzhydryl alcohol
Inchi:	InChI=1S/C13H11BrO/c14-12-8-6-11(7-9-12)13(15)10-4-2-1-3-5-10/h1-9,13,15H
InchiKey:	WTIWDBNPPSHSCB-UHFFFAOYSA-N
Formula:	C13H11BrO
SMILES:	OC(c1ccccc1)c1ccc(Br)cc1
Mol. weight [g/mol]:	263.13
CAS:	29334-16-5

Physical Properties

Property code	Value	Unit	Source
gf	148.83	kJ/mol	Joback Method
hf	18.76	kJ/mol	Joback Method
hfus	22.97	kJ/mol	Joback Method
hvap	72.47	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.531		Crippen Method
mcvol	169.880	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	713.08	K	Joback Method
tc	953.11	K	Joback Method
tf	407.25	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.17	J/mol×K	713.08	Joback Method
cpg	423.93	J/mol×K	753.08	Joback Method
cpg	434.72	J/mol×K	793.09	Joback Method

cpg	444.62	J/mol×K	833.09	Joback Method
cpg	453.72	J/mol×K	873.10	Joback Method
cpg	462.10	J/mol×K	913.10	Joback Method
cpg	469.84	J/mol×K	953.11	Joback Method
dvisc	0.0018391	Pa×s	407.25	Joback Method
dvisc	0.0006894	Pa×s	458.22	Joback Method
dvisc	0.0003145	Pa×s	509.19	Joback Method
dvisc	0.0001655	Pa×s	560.16	Joback Method
dvisc	0.0000970	Pa×s	611.14	Joback Method
dvisc	0.0000617	Pa×s	662.11	Joback Method
dvisc	0.0000418	Pa×s	713.08	Joback Method

Sources

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=C29334165&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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