

Benzene, 1-bromo-4-(2-phenylethyl)-

Other names:	Bibenzyl, 4-bromo-4-Bromobibenzyl 1-(4-Bromophenyl)-2-phenylethane
Inchi:	InChI=1S/C14H13Br/c15-14-10-8-13(9-11-14)7-6-12-4-2-1-3-5-12/h1-5,8-11H,6-7H2
InchiKey:	FTRWFZZSIXRXFI-UHFFFAOYSA-N
Formula:	C14H13Br
SMILES:	<chem>Brc1ccc(CCc2ccccc2)cc1</chem>
Mol. weight [g/mol]:	261.16
CAS:	14310-24-8

Physical Properties

Property code	Value	Unit	Source
gf	296.51	kJ/mol	Joback Method
hf	155.63	kJ/mol	Joback Method
hfus	24.99	kJ/mol	Joback Method
hvap	58.41	kJ/mol	Joback Method
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-5.05		Crippen Method
logp	4.234		Crippen Method
mcvol	178.100	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
tb	644.22	K	Joback Method
tc	897.53	K	Joback Method
tf	372.70	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.46	J/molxK	644.22	Joback Method
cpg	478.79	J/molxK	855.31	Joback Method
cpg	467.71	J/molxK	813.09	Joback Method
cpg	455.63	J/molxK	770.87	Joback Method
cpg	442.46	J/molxK	728.66	Joback Method

cpg	428.10	J/molxK	686.44	Joback Method
cpg	488.98	J/molxK	897.53	Joback Method
dvisc	0.0001733	Paxs	644.22	Joback Method
dvisc	0.0002173	Paxs	598.97	Joback Method
dvisc	0.0002827	Paxs	553.71	Joback Method
dvisc	0.0003855	Paxs	508.46	Joback Method
dvisc	0.0005585	Paxs	463.21	Joback Method
dvisc	0.0008766	Paxs	417.95	Joback Method
dvisc	0.0015353	Paxs	372.70	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=C14310248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ie:	Ionization energy
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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