

4-Benzyloxybromobenzene

Other names:	Benzene, 1-bromo-4-(phenylmethoxy)-
Inchi:	InChI=1S/C13H11BrO/c14-12-6-8-13(9-7-12)15-10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey:	OUQSGILAXUXMGI-UHFFFAOYSA-N
Formula:	C13H11BrO
SMILES:	<chem>Brc1ccc(OCc2ccccc2)cc1</chem>
Mol. weight [g/mol]:	263.13
CAS:	6793-92-6

Physical Properties

Property code	Value	Unit	Source
gf	183.09	kJ/mol	Joback Method
hf	44.05	kJ/mol	Joback Method
hfus	23.59	kJ/mol	Joback Method
hvap	58.59	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.028		Crippen Method
mcvol	169.880	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	643.76	K	Joback Method
tc	898.55	K	Joback Method
tf	383.66	K	Joback Method
vc	0.627	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.60	J/molxK	643.76	Joback Method
cpg	402.21	J/molxK	686.22	Joback Method
cpg	415.62	J/molxK	728.69	Joback Method
cpg	427.90	J/molxK	771.15	Joback Method
cpg	439.11	J/molxK	813.62	Joback Method
cpg	449.33	J/molxK	856.08	Joback Method
cpg	458.63	J/molxK	898.55	Joback Method
dvisc	0.0011903	Paxs	383.66	Joback Method

dvisc	0.0007092	Paxs	427.01	Joback Method
dvisc	0.0004649	Paxs	470.36	Joback Method
dvisc	0.0003272	Paxs	513.71	Joback Method
dvisc	0.0002433	Paxs	557.06	Joback Method
dvisc	0.0001888	Paxs	600.41	Joback Method
dvisc	0.0001516	Paxs	643.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C6793926&Units=SI

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
mccvol:	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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