

4-Bromoguaiacol

Other names:	Phenol, 4-bromo-2-methoxy- 4-Bromo-2-methoxyphenol
Inchi:	InChI=1S/C7H7BrO2/c1-10-7-4-5(8)2-3-6(7)9/h2-4,9H,1H3
InchiKey:	WHSIIJQOEGXWSN-UHFFFAOYSA-N
Formula:	C7H7BrO2
SMILES:	COc1cc(Br)ccc1O
Mol. weight [g/mol]:	203.03
CAS:	7368-78-7

Physical Properties

Property code	Value	Unit	Source
gf	-134.46	kJ/mol	Joback Method
hf	-245.95	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	55.97	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.163		Crippen Method
mcvol	114.970	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
rinpol	1388.10		NIST Webbook
rinpol	1388.10		NIST Webbook
tb	560.42	K	Joback Method
tc	804.58	K	Joback Method
tf	401.34	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.21	J/molxK	560.42	Joback Method
cpg	244.27	J/molxK	601.11	Joback Method
cpg	252.65	J/molxK	641.81	Joback Method
cpg	260.43	J/molxK	682.50	Joback Method
cpg	267.69	J/molxK	723.19	Joback Method

cpg	274.49	J/mol×K	763.89	Joback Method
cpg	280.92	J/mol×K	804.58	Joback Method
dvisc	0.0008506	Paxs	401.34	Joback Method
dvisc	0.0004679	Paxs	427.85	Joback Method
dvisc	0.0002760	Paxs	454.37	Joback Method
dvisc	0.0001725	Paxs	480.88	Joback Method
dvisc	0.0001133	Paxs	507.39	Joback Method
dvisc	0.0000775	Paxs	533.91	Joback Method
dvisc	0.0000550	Paxs	560.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7368787&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

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