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/mol×K	560.42	Joback Method
cpg	274.49	J/mol×K	763.89	Joback Method
cpg	267.69	J/mol×K	723.19	Joback Method
cpg	260.43	J/mol×K	682.50	Joback Method
cpg	252.65	J/mol×K	641.81	Joback Method

cpg	244.27	J/mol×K	601.11	Joback Method
cpg	280.92	J/mol×K	804.58	Joback Method
dvisc	0.0000550	Pa×s	560.42	Joback Method
dvisc	0.0000775	Pa×s	533.91	Joback Method
dvisc	0.0001133	Pa×s	507.39	Joback Method
dvisc	0.0001725	Pa×s	480.88	Joback Method
dvisc	0.0002760	Pa×s	454.37	Joback Method
dvisc	0.0004679	Pa×s	427.85	Joback Method
dvisc	0.0008506	Pa×s	401.34	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/ci990307l
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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