Phenol, 4-bromo-2-methoxy-

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]: 203.04

Physical Properties

Property code	Value	Unit	Source
hf	-212.01	kJ/mol	Cheméo Relay (1.0)
hfus	19.79	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Cheméo Relay (1.0)
ie	8.16	eV	Cheméo Relay (1.0)
log10ws	-2.33		Cheméo Relay (1.0)
logp	2.163		Crippen Method
mcvol	114.970	ml/mol	McGowan Method
rinpol	1388.10		NIST Webbook
rinpol	1388.10		NIST Webbook
tb	525.93	K	Cheméo Relay (1.0)
tf	332.44	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.21	J/mol×K	560.42	Joback Method
cpg	280.92	J/mol×K	804.58	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
dvisc	0.0001725	Pa×s	480.88	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	0.0008506	Pa×s	401.34	Joback Method
dvisc	0.0002760	Pa×s	454.37	Joback Method
dvisc	0.0004679	Pa×s	427.85	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7368787&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point