Phenol, 2-bromo-4-methyl-

Other names:	2-Bromo-p-cresol
	3-Bromo-4-hydroxytoluene
	2-Bromo-4-methylphenol
	p-Cresol, 2-bromo-
Inchi:	InChI=1S/C7H7BrO/c1-5-2-3-7(9)6(8)4-5/h2-4,9H,1H3
InchiKey:	MTIDYGLTAOZOGU-UHFFFAOYSA-N
Formula:	C7H7BrO
SMILES:	Cc1ccc(O)c(Br)c1
Mol. weight [g/mol]:	187.03
CAS:	6627-55-0

Physical Properties

Property code	Value	Unit	Source
gf	-29.46	kJ/mol	Joback Method
hf	-113.73	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	53.56	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.463		Crippen Method
mcvol	109.100	ml/mol	McGowan Method
pc	5438.52	kPa	Joback Method
rinpol	1153.50		NIST Webbook
rinpol	1153.50		NIST Webbook
tb	486.70	K	NIST Webbook
tc	785.86	K	Joback Method
tf	328.00 ± 0.50	K	NIST Webbook
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.81	J/mol×K	538.00	Joback Method
cpg	253.95	J/mol×K	744.55	Joback Method
cpg	247.30	J/mol×K	703.24	Joback Method

cpg	240.16	J/mol×K	661.93	Joback Method
cpg	232.44	J/mol×K	620.62	Joback Method
cpg	224.02	J/mol×K	579.31	Joback Method
cpg	260.21	J/mol×K	785.86	Joback Method
dvisc	0.0000793	Pa×s	538.00	Joback Method
dvisc	0.0001137	Pa×s	511.52	Joback Method
dvisc	0.0001696	Pa×s	485.04	Joback Method
dvisc	0.0002651	Pa×s	458.56	Joback Method
dvisc	0.0004376	Pa×s	432.07	Joback Method
dvisc	0.0007711	Pa×s	405.59	Joback Method
dvisc	0.0014707	Pa×s	379.11	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=C6627550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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