Phenol, 4-bromo-2,6-dimethyl-

Other names: 4-Bromo-2,6-dimethylphenol
2,6-Xylenol, 4-bromo-
4-Bromo-2,6-xylenol
Inchi: InChI=1S/C8H9BrO/c1-5-3-7(9)4-6(2)8(5)10/h3-4,10H,1-2H3
InchiKey: ZLVFYUORUHNMBO-UHFFFAOYSA-N
Formula: C8H9BrO
SMILES: Cc1cc(Br)cc(C)c1O
Mol. weight [g/mol]: 201.06
CAS: 2374-05-2

Physical Properties

Property code	Value	Unit	Source
gf	-30.67	kJ/mol	Joback Method
hf	-145.84	kJ/mol	Joback Method
hfus	20.81	kJ/mol	Joback Method
hvap	56.45	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.772		Crippen Method
mcvol	123.190	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	565.86	K	Joback Method
tc	809.66	K	Joback Method
tf	402.90	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.30	J/mol×K	565.86	Joback Method
cpg	266.32	J/mol×K	606.49	Joback Method
cpg	275.61	J/mol×K	647.13	Joback Method
cpg	284.26	J/mol×K	687.76	Joback Method
cpg	292.35	J/mol×K	728.40	Joback Method
cpg	299.97	J/mol×K	769.03	Joback Method

cpg	307.22	J/mol×K	809.66	Joback Method
dvisc	0.0008830	Pa×s	402.90	Joback Method
dvisc	0.0004873	Pa×s	430.06	Joback Method
dvisc	0.0002886	Pa×s	457.22	Joback Method
dvisc	0.0001813	Pa×s	484.38	Joback Method
dvisc	0.0001196	Pa×s	511.54	Joback Method
dvisc	0.0000823	Pa×s	538.70	Joback Method
dvisc	0.0000587	Pa×s	565.86	Joback Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2374052&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
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume