3,5-Dibromo-4-methylphenol

Other names:	Phenol, 3,5-dibromo-4-methyl- 3,5-dibromo-p-cresol
Inchi:	InChI=1S/C7H6Br2O/c1-4-6(8)2-5(10)3-7(4)9/h2-3,10H,1H3
InchiKey:	AXCQKKVGMZCWPC-UHFFFAOYSA-N
Formula:	C7H6Br2O
SMILES:	Cc1c(Br)cc(O)cc1Br
Mol. weight [g/mol]:	265.93
CAS:	13979-81-2

Physical Properties

Property code	Value	Unit	Source
gf	-24.77	kJ/mol	Joback Method
hf	-98.87	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.226		Crippen Method
mcvol	126.600	ml/mol	McGowan Method
pc	5899.00	kPa	Joback Method
tb	609.14	K	Joback Method
tc	872.28	K	Joback Method
tf	451.43	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.15	J/mol×K	609.14	Joback Method
cpg	247.83	J/mol×K	653.00	Joback Method
cpg	254.87	J/mol×K	696.85	Joback Method
cpg	261.41	J/mol×K	740.71	Joback Method
cpg	267.56	J/mol×K	784.57	Joback Method
cpg	273.45	J/mol×K	828.42	Joback Method
cpg	279.21	J/mol×K	872.28	Joback Method

dvisc	0.0004708	Pa×s	451.43	Joback Method
dvisc	0.0002897	Pa×s	477.72	Joback Method
dvisc	0.0001876	Pa×s	504.00	Joback Method
dvisc	0.0001268	Pa×s	530.28	Joback Method
dvisc	0.0000889	Pa×s	556.57	Joback Method
dvisc	0.0000644	Pa×s	582.86	Joback Method
dvisc	0.0000479	Pa×s	609.14	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=C13979812&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