

4,6-Dibromo-o-cresol

Other names:	o-Cresol, 4,6-dibromo-
Inchi:	InChI=1S/C7H6Br2O/c1-4-2-5(8)3-6(9)7(4)10/h2-3,10H,1H3
InchiKey:	XMKVPKGUYUXVWEB-UHFFFAOYSA-N
Formula:	C7H6Br2O
SMILES:	Cc1cc(Br)cc(Br)c1O
Mol. weight [g/mol]:	265.93
CAS:	609-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-24.77	kJ/mol	Joback Method
hf	-98.87	kJ/mol	Joback Method
hfs	-159.00 ± 6.00	kJ/mol	NIST Webbook
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/molxK	609.14	Joback Method
cpg	247.83	J/molxK	653.00	Joback Method
cpg	254.87	J/molxK	696.85	Joback Method
cpg	261.41	J/molxK	740.71	Joback Method
cpg	267.56	J/molxK	784.57	Joback Method
cpg	273.45	J/molxK	828.42	Joback Method
cpg	279.21	J/molxK	872.28	Joback Method

dvisc	0.0004708	Paxs	451.43	Joback Method
dvisc	0.0002897	Paxs	477.72	Joback Method
dvisc	0.0001876	Paxs	504.00	Joback Method
dvisc	0.0001268	Paxs	530.28	Joback Method
dvisc	0.0000889	Paxs	556.57	Joback Method
dvisc	0.0000644	Paxs	582.86	Joback Method
dvisc	0.0000479	Paxs	609.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

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