

p-Benzoquinone, 2,5-dibromo-3,6-dihydroxy-

Other names:	Bromanilic acid 2,5-Cyclohexadiene-1,4-dione, 2,5-dibromo-3,6-dihydroxy- 2,5-Dibromo-3,6-dihydroxyquinone 2,5-Dibromo-3,6-dihydroxy-p-benzoquinone
Inchi:	InChI=1S/C6H2Br2O4/c7-1-3(9)5(11)2(8)6(12)4(1)10/h9,12H
InchiKey:	GMZWPTALVQRAFV-UHFFFAOYSA-N
Formula:	C6H2Br2O4
SMILES:	O=C1C(O)=C(Br)C(=O)C(O)=C1Br
Mol. weight [g/mol]:	297.89
CAS:	4370-59-6

Physical Properties

Property code	Value	Unit	Source
gf	-436.98	kJ/mol	Joback Method
hf	-550.03	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.467		Crippen Method
mcvol	125.820	ml/mol	McGowan Method
pc	7535.20	kPa	Joback Method
tb	831.46	K	Joback Method
tc	1066.95	K	Joback Method
tf	598.28	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.86	J/molxK	831.46	Joback Method
cpg	274.01	J/molxK	870.71	Joback Method
cpg	278.53	J/molxK	909.96	Joback Method
cpg	282.38	J/molxK	949.21	Joback Method
cpg	285.50	J/molxK	988.45	Joback Method

cpg	287.84	J/mol×K	1027.70	Joback Method
cpg	289.37	J/mol×K	1066.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4370596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
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

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