2,5-CYCLOHEXADIENE-1,4-DIONE, 2,5-DIBROMO-3,6-DIHYDROXY-

Other names: 2,5-Cyclohexadiene-1,4-dione, 2,5-dibromo-3,6-dihydroxy-
2,5-Dibromo-3,6-dihydroxy-p-benzoquinone
2,5-Dibromo-3,6-dihydroxyquinone
Bromanilic acid

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

Physical Properties

Property code	Value	Unit	Source
hfus	20.71	kJ/mol	Joback Method
ie	9.57	eV	Cheméo Relay (1.0)
logp	1.467		Crippen Method
mcvol	125.820	ml/mol	McGowan Method

Temperature Dependent Properties

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

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4370596&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume