1(3H)-Isobenzofuranone, 3,3-bis(3,5-dibromo-4-hydroxyphenyl)-

Other names: Phenolphthalein, 3',3'',5',5''-tetrabromo-
Tetrabromophenolphthalein
3',3'',5',5''-Tetrabromophenolphthalein
3,3-bis(3,5-dibromo-4-hydroxyphenyl)phthalide

Inchi: InChI=1S/C20H10Br4O4/c21-13-5-9(6-14(22)17(13)25)20(10-7-15(23)18(26)16(24)8-10)

InchiKey: OBRGVMYQZVQHGO-UHFFFAOYSA-N

Formula: C20H10Br4O4

SMILES: O=C1OC(c2cc(Br)c(O)c(Br)c2)(c2cc(Br)c(O)c(Br)c2)c2ccccc21

Mol. weight [g/mol]: 633.91

CAS: 76-62-0

Physical Properties

Property code	Value	Unit	Source
gf	1.19	kJ/mol	Joback Method
hf	-234.85	kJ/mol	Joback Method
hfus	59.77	kJ/mol	Joback Method
hvap	129.54	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	6.610		Crippen Method
mcvol	299.700	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
tb	1289.57	K	Joback Method
tc	1612.31	K	Joback Method
tf	1056.29	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.31	J/mol×K	1289.57	Joback Method
cpg	1007.49	J/mol×K	1343.36	Joback Method
cpg	1068.41	J/mol×K	1397.15	Joback Method
cpg	1137.88	J/mol×K	1450.94	Joback Method
cpg	1216.68	J/mol×K	1504.73	Joback Method

cpg	1305.63	J/mol×K	1558.52	Joback Method
cpg	1405.53	J/mol×K	1612.31	Joback Method

Sources

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=C76620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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