4-[3-(4-hydroxyphenyl)-1,1-dioxobenzo[c]oxathiol

Inchi: InChI=1S/C19H14O5S/c20-15-9-5-13(6-10-15)19(14-7-11-16(21)12-8-14)17-3-1-2-4-18(
InchiKey: BELBBZDIHDAJOR-UHFFFAOYSA-N
Formula: C19H14O5S
SMILES: O=S1(=O)OC(c2ccc(O)cc2)(c2ccc(O)cc2)c2ccccc21
Mol. weight [g/mol]: 354.38

Physical Properties

Property code	Value	Unit	Source
gf	-365.20	kJ/mol	Joback Method
hf	-585.91	kJ/mol	Joback Method
hfus	48.99	kJ/mol	Joback Method
hvap	112.31	kJ/mol	Joback Method
log10ws	-3.07		Aqueous Solubility Prediction Method
logp	3.109		Crippen Method
mcvol	242.130	ml/mol	McGowan Method
pc	4640.32	kPa	Joback Method
tb	941.14	K	Joback Method
tc	1215.23	K	Joback Method
tf	775.13	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.88	J/mol×K	941.14	Joback Method
cpg	755.66	J/mol×K	986.82	Joback Method
cpg	775.97	J/mol×K	1032.50	Joback Method
cpg	798.33	J/mol×K	1078.19	Joback Method
cpg	823.24	J/mol×K	1123.87	Joback Method
cpg	851.21	J/mol×K	1169.55	Joback Method
cpg	882.77	J/mol×K	1215.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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