Benzonitrile, 4-hydroxy-3,5-diiodo-

Other names:	2,6-Diiodo-4-cyanophenol
	3,5-Diiodo-4-hydroxybenzonitrile
	3,5-Dijod-4-hydroxy-benzonitril
	4-Cyano-2,6-diiodophenol
	4-Cyano-2,6-dijodphenol
	4-Hydroxy-3,5-diiodobenzonitrile
	ACP 63303
	Actril
	Bantrol
	Bentrol
	Benzonitrile, 3,5-diiodo-4-hydroxy-
	Ca 69-15
	Certol
	Certrol
	Cipotril
	Iotox
	Ioxinyl
	Ioxynil
	Joxynil
	M&B 8873
	Totril
	Trevespan
Inchi:	InChI=1S/C7H3I2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H
InchiKey:	NRXQIUSYPAHGNM-UHFFFAOYSA-N
Formula:	C7H3I2NO
SMILES:	N#Cc1cc(I)c(O)c(I)c1
Mol. weight [g/mol]:	370.91

Physical Properties

Property code	Value	Unit	Source
chs	-3219.00	kJ/mol	NIST Webbook
hfs	-1.90	kJ/mol	NIST Webbook
hfus	23.25	kJ/mol	Joback Method
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-3.61		Aqueous Solubility Prediction Method

log10ws	-3.61		Estimated Solubility Method
logp	2.473		Crippen Method
mcvol	144.620	ml/mol	McGowan Method
rinpol	1927.00		NIST Webbook
tf	481.40	K	Aqueous Solubility Prediction Method
tf	488.91 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.01	J/mol×K	765.18	Joback Method
cpg	254.13	J/mol×K	816.43	Joback Method
cpg	259.16	J/mol×K	867.69	Joback Method
cpg	264.28	J/mol×K	918.94	Joback Method
cpg	269.72	J/mol×K	970.20	Joback Method
cpg	275.67	J/mol×K	1021.45	Joback Method
cpg	282.34	J/mol×K	1072.71	Joback Method
hfust	33.63	kJ/mol	482.90	NIST Webbook
hfust	33.63	kJ/mol	482.90	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1689834&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point