Benzonitrile, 3,5-dibromo-4-hydroxy-

Other names:	2,6-Dibromo-4-cyanophenol
	3,5-Dibromo-4-hydroxybenzonitrile
	3,5-Dibromo-4-hydroxyphenylcyanide
	4-Cyano-2,6-dibromophenol
	4-Hydroxy-3,5-dibromobenzonitrile
	Brittox
	Brominal
	Brominex
	Brominil
	Bromotril
	Broxynil
	Bucril
	Buctril
	Buctril industrial
	Butilchlorofos
	Certrol B
	Chipco buctril
	Chipco crab-kleen
	ENT 20852
	Labuctril
	Labuctril 25
	Litarol M
	M&B 10,064
	M&B 10731
	MB 10064
	ME4 Brominal
	Nu-lawn weeder
	Oxytril M
	Pardner
	S 2132
	Sabre
	Toplan
	Torch
	bromoxynil
Inchi:	InChI=1S/C7H3Br2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H
InchiKey:	UPMXNNIRAGDFEH-UHFFFAOYSA-N
Formula:	C7H3Br2NO
SMILES:	N#Cc1cc(Br)c(O)c(Br)c1
Mol. weight [g/mol]:	276.91

Physical Properties

Property code	Value	Unit	Source
hf	100.46	kJ/mol	Cheméo Relay (1.0)
hfus	25.01	kJ/mol	Joback Method
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-3.33		Estimated Solubility Method
log10ws	-3.33		Aqueous Solubility Prediction Method
logp	2.789		Crippen Method
mcvol	127.980	ml/mol	McGowan Method
rinpol	1686.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	547.36	K	Cheméo Relay (1.0)
tf	463.60 ± 0.20	K	NIST Webbook
tf	464.20 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.09	J/mol×K	711.22	Joback Method
cpg	246.39	J/mol×K	756.97	Joback Method
cpg	251.39	J/mol×K	802.73	Joback Method
cpg	256.23	J/mol×K	848.48	Joback Method
cpg	261.05	J/mol×K	894.23	Joback Method
cpg	266.00	J/mol×K	939.98	Joback Method
cpg	271.20	J/mol×K	985.74	Joback Method
hfust	32.03	kJ/mol	464.00	NIST Webbook
hfust	32.03	kJ/mol	464.00	NIST Webbook

Sources

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
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=C1689845&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point