

5-Chloro-7-bromo-8-hydroxyquinoline

Other names:	7-Bromo-5-chloro-8-hydroxyquinoline 8-Quinolinol, 7-bromo-5-chloro- 5-Chlor-7-brom-8-hydroxychinolin 7-bromo-5-chloroquinolin-8-ol
Inchi:	InChI=1S/C9H5BrClNO/c10-6-4-7(11)5-2-1-3-12-8(5)9(6)13/h1-4,13H
InchiKey:	ADJQQSUBKRASQN-UHFFFAOYSA-N
Formula:	C9H5BrClNO
SMILES:	Oc1c(Br)cc(Cl)c2cccnc12
Mol. weight [g/mol]:	258.50
CAS:	7640-33-7

Physical Properties

Property code	Value	Unit	Source
chs	-4130.20 ± 1.70	kJ/mol	NIST Webbook
hf	-14.50 ± 2.20	kJ/mol	NIST Webbook
hfs	-127.70 ± 2.10	kJ/mol	NIST Webbook
hsub	113.20 ± 0.80	kJ/mol	NIST Webbook
log10ws	-4.44		Crippen Method
logp	3.356		Crippen Method
mcvol	140.040	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	110.10 ± 0.80	kJ/mol	360.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7640337&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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