

Broxyquinoline

Other names:	5,7-Dibromo-8-hydroxyquinoline
	5,7-Dibromo-8-quinolinol
	5,7-Dibromooxine
	5,7-Dibromoquinolin-8-ol
	8-Quinolinol, 5,7-dibromo-
	Brodiar
	Broxiquinoline
	Broxykinolin
	Broxyquinolin
	Colepur
	Colipar
	Dibromoksin
	Dibromoquin
	Dibromoxin
	Dibromoxine
	Dibromoxyquinoline
	Fenilor
	Intensopan
	NSC 1810
	Paramiba
	Paramibe
Inchi:	InChI=1S/C9H5Br2NO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H
InchiKey:	ZDASUJMDVPTNTF-UHFFFAOYSA-N
Formula:	C9H5Br2NO
SMILES:	Oc1c(Br)cc(Br)c2cccnc12
Mol. weight [g/mol]:	302.95
CAS:	521-74-4

Physical Properties

Property code	Value	Unit	Source
chs	-4171.90 ± 2.50	kJ/mol	NIST Webbook
hf	76.80 ± 3.10	kJ/mol	NIST Webbook
hfs	-40.50 ± 2.80	kJ/mol	NIST Webbook
hsub	117.30 ± 1.30	kJ/mol	NIST Webbook
hsub	94.10 ± 0.80	kJ/mol	NIST Webbook
log10ws	-4.92		Crippen Method

logp	3.465		Crippen Method
mvol	145.300	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	113.60 ± 1.30	kJ/mol	372.50	NIST Webbook
hsubt	94.10	kJ/mol	378.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.23696e+01
Coeff. B	-1.13057e+04
Temperature range (K), min.	511.99
Temperature range (K), max.	662.77

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C521744&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
pvap:	Vapor pressure

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