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
hvap	93.48	kJ/mol	Cheméo Relay (1.0)

ie	8.31	eV	Cheméo Relay (1.0)
log10ws	-3.65		Cheméo Relay (1.0)
logp	3.465		Crippen Method
mcvol	145.300	ml/mol	McGowan Method
tf	394.63	K	Cheméo Relay (1.0)

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(Pvp) = 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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C521744&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tf:	Normal melting (fusion) point