

Phenol, 4-amino-2,6-dibromo-

Other names:	4-Amino-2,6-dibromophenol 2,6-Dibromo-4-aminophenol 3,5-Dibromo-4-hydroxyaniline
Inchi:	InChI=1S/C6H5Br2NO/c7-4-1-3(9)2-5(8)6(4)10/h1-2,10H,9H2
InchiKey:	HFYPXERYZGFDBD-UHFFFAOYSA-N
Formula:	C6H5Br2NO
SMILES:	Nc1cc(Br)c(O)c(Br)c1
Mol. weight [g/mol]:	266.92
CAS:	609-21-2

Physical Properties

Property code	Value	Unit	Source
gf	33.26	kJ/mol	Joback Method
hf	-44.44	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	69.08	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.499		Crippen Method
mcvol	122.490	ml/mol	McGowan Method
pc	7574.60	kPa	Joback Method
tb	658.79	K	Joback Method
tc	934.12	K	Joback Method
tf	523.42	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.89	J/molxK	658.79	Joback Method
cpg	245.28	J/molxK	704.68	Joback Method
cpg	251.18	J/molxK	750.57	Joback Method
cpg	256.72	J/molxK	796.46	Joback Method
cpg	262.06	J/molxK	842.34	Joback Method
cpg	267.33	J/molxK	888.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609212&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/96-879-1/Phenol-4-amino-2-6-dibromo.pdf>

Generated by Cheméo on 2024-04-26 16:16:53.690993718 +0000 UTC m=+16437462.611571029.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.