2,4-Dibromoaniline

Other names:	2,4-Dibromoaniline
	2,4-Dibromanilin
	NSC 88324
Inchi:	InChI=1S/C6H5Br2N/c7-4-1-2-6(9)5(8)3-4/h1-3H,9H2
InchiKey:	DYSRXWYRUJCNFI-UHFFFAOYSA-N
Formula:	C6H5Br2N
SMILES:	Nc1ccc(Br)cc1Br
Mol. weight [g/mol]:	250.92

Physical Properties

Property code	Value	Unit	Source
hf	139.00	kJ/mol	Cheméo Relay (1.0)
hfus	20.33	kJ/mol	Joback Method
hsub	88.00 ± 1.50	kJ/mol	NIST Webbook
hvap	71.37	kJ/mol	Cheméo Relay (1.0)
ie	7.93	eV	Cheméo Relay (1.0)
log10ws	-2.96		Cheméo Relay (1.0)
logp	2.794		Crippen Method
mcvol	116.620	ml/mol	McGowan Method
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
tb	550.16	K	Cheméo Relay (1.0)
tf	341.21	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.53	J/mol×K	578.17	Joback Method
cpg	213.33	J/mol×K	622.64	Joback Method
cpg	220.45	J/mol×K	667.11	Joback Method
cpg	226.96	J/mol×K	711.58	Joback Method
cpg	232.91	J/mol×K	756.05	Joback Method
cpg	238.36	J/mol×K	800.52	Joback Method

cpg	243.39	J/mol×K	844.98	Joback Method
hfust	21.37	kJ/mol	351.40	NIST Webbook

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615576&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
hsub: Enthalpy of sublimation at standard conditions
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point