

Cyanogen bromide

Other names:	(CN)Br BrCN Bromine cyanide Bromine cyanide (BrCN) Bromine monocyanoide Bromocyan Bromocyanide Bromocyanide (BrCN) Bromocyanogen Bromure de cyanogen Campilit Cyanobromide Cyanogen bromide ((CN)Br) Cyanogen bromide (BrCN) Cyanogen monobromide NSC 89684 Rcra waste number U246 TL 822 UN 1889
Inchi:	InChI=1S/CBrN/c2-1-3
InchiKey:	ATDGTVJJHBUTRL-UHFFFAOYSA-N
Formula:	CBrN
SMILES:	N#CBr
Mol. weight [g/mol]:	105.92
CAS:	506-68-3

Physical Properties

Property code	Value	Unit	Source
affp	749.80	kJ/mol	NIST Webbook
basg	719.20	kJ/mol	NIST Webbook
gf	105.04	kJ/mol	Joback Method
hf	185.60 ± 6.00	kJ/mol	NIST Webbook
hfs	140.40 ± 4.30	kJ/mol	NIST Webbook
hfus	5.14	kJ/mol	Joback Method
hsub	45.23	kJ/mol	NIST Webbook
hvap	34.73	kJ/mol	Joback Method
ie	11.85 ± 0.02	eV	NIST Webbook

ie	11.84 ± 0.01	eV	NIST Webbook
ie	12.00 ± 1.00	eV	NIST Webbook
ie	11.88	eV	NIST Webbook
log10ws	-1.03		Crippen Method
logp	0.862		Crippen Method
mvol	43.830	ml/mol	McGowan Method
pc	6200.01	kPa	Joback Method
rinpol	482.00		NIST Webbook
rinpol	482.00		NIST Webbook
tb	390.52	K	Joback Method
tc	609.48	K	Joback Method
tf	225.82	K	Joback Method
vc	0.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	48.88	J/mol×K	500.00	Joback Method
cpg	49.66	J/mol×K	536.49	Joback Method
cpg	50.36	J/mol×K	572.99	Joback Method
cpg	46.08	J/mol×K	390.52	Joback Method
cpg	47.10	J/mol×K	427.01	Joback Method
cpg	48.03	J/mol×K	463.51	Joback Method
cpg	51.01	J/mol×K	609.48	Joback Method
hsubt	45.20 ± 4.20	kJ/mol	290.50	NIST Webbook
hsubt	45.90	kJ/mol	293.00	NIST Webbook
hsubt	47.00	kJ/mol	282.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56682e+01
Coeff. B	-2.78893e+03
Coeff. C	-8.21550e+01
Temperature range (K), min.	260.15
Temperature range (K), max.	351.57

Sources

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=C506683&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/ci9903071

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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