

Boron trifluoride

Other names:	Anca 1040 BF3 BORON FLUORIDE Borane, trifluoro- Boron fluoride (BF3) Fluorure de bore TRIFLUOROBORANE Trifluoroboron UN 1008
Inchi:	InChI=1S/BF3/c2-1(3)4
InchiKey:	WTEOIRVLGSZEPR-UHFFFAOYSA-N
Formula:	BF3
SMILES:	FB(F)F
Mol. weight [g/mol]:	67.81
CAS:	7637-07-2

Physical Properties

Property code	Value	Unit	Source
af	0.3930		KDB
dm	0.00	debye	KDB
ea	2.65	eV	NIST Webbook
gf	-1120.00	kJ/mol	KDB
hf	-1136.00 ± 0.80	kJ/mol	NIST Webbook
hf	-1136.00	kJ/mol	KDB
ie	15.25	eV	NIST Webbook
ie	15.96	eV	NIST Webbook
ie	16.00	eV	NIST Webbook
ie	15.55 ± 0.04	eV	NIST Webbook
ie	15.57 ± 0.02	eV	NIST Webbook
ie	15.71 ± 0.10	eV	NIST Webbook
ie	15.70 ± 0.30	eV	NIST Webbook
ie	15.95	eV	NIST Webbook
ie	15.94	eV	NIST Webbook
ie	15.50	eV	NIST Webbook
ie	15.96 ± 0.01	eV	NIST Webbook
ie	16.00 ± 1.00	eV	NIST Webbook
log10ws	1.37		Crippen Method

logp	0.880		Crippen Method
pc	4980.00	kPa	KDB
sgb	254.42 ± 0.20	J/mol×K	NIST Webbook
tb	172.00	K	KDB
tc	260.80	K	KDB
tf	146.30	K	KDB
vc	0.115	m ³ /kmol	KDB
zc	0.2641090		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhoI	2811.00	kg/m ³	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47734e+01
Coeff. B	-1.42384e+03
Coeff. C	-3.31400e+01
Temperature range (K), min.	144.78
Temperature range (K), max.	260.90

Sources

Crippen Method:

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

KDB:

<https://www.thermochimica.org/files/research/kdb/mol/mol1894.mol>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C7637072&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

af:	Acentric Factor
dm:	Dipole Moment
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
sgb:	Molar entropy at standard conditions (1 bar)
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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