Bromotrifluoromethane

Other names:	Bromofluoroform
	CBrF3
	CF3Br
	Carbon monobromide trifluoride
	Daiflon 13B1
	F 13B1
	FC 13B1
	Flugex 13B1
	Fluorocarbon 1301
	Freon 13B1
	Halon 1301
	Khladon 13B1
	Methane, bromotrifluoro-
	Monobromotrifluoromethane
	R 13B1
	Refrigerant 13B1
	Trifluorobromomethane
	Trifluoromethyl bromide
	Trifluoromonobromomethane
	UN 1009
Inchi:	InChI=1S/CBrF3/c2-1(3,4)5
InchiKey:	RJCQBQGAPKAMLL-UHFFFAOYSA-N
Formula:	CBrF3
SMILES:	FC(F)(F)Br
Mol. weight [g/mol]:	148.91
CAS:	75-63-8

Physical Properties

Property code	Value	Unit	Source
affp	580.00	kJ/mol	NIST Webbook
basg	550.30	kJ/mol	NIST Webbook
ea	0.91 ± 0.20	eV	NIST Webbook
gf	-609.73	kJ/mol	Joback Method
hf	-647.30 ± 2.90	kJ/mol	NIST Webbook
hf	-649.40 ± 3.20	kJ/mol	NIST Webbook
hfus	5.46	kJ/mol	Joback Method
hvap	20.51	kJ/mol	Joback Method

ie	11.70	eV	NIST Webbook
ie	11.76 ± 0.02	eV	NIST Webbook
ie	11.40 ± 0.01	eV	NIST Webbook
ie	11.82 ± 0.02	eV	NIST Webbook
ie	11.89 ± 0.10	eV	NIST Webbook
ie	12.30 ± 0.30	eV	NIST Webbook
ie	12.40	eV	NIST Webbook
ie	12.08 ± 0.05	eV	NIST Webbook
ie	11.40 ± 0.01	eV	NIST Webbook
ie	12.00	eV	NIST Webbook
ie	12.12 ± 0.02	eV	NIST Webbook
ie	12.10	eV	NIST Webbook
log10ws	-1.83		Crippen Method
logp	1.901		Crippen Method
mcvol	47.760	ml/mol	McGowan Method
pc	3956.00 ± 3.00	kPa	NIST Webbook
rhoc	763.91 ± 4.47	kg/m3	NIST Webbook
rinpol	222.00		NIST Webbook
rinpol	222.00		NIST Webbook
tb	215.30	K	NIST Webbook
tc	340.08 ± 0.02	K	NIST Webbook
tf	98.47 ± 0.05	K	NIST Webbook
tf	98.72 ± 0.05	K	NIST Webbook
vc	0.197	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	75.81	J/mol×K	365.21	Joback Method
cpg	78.73	J/mol×K	392.60	Joback Method
cpg	81.39	J/mol×K	420.00	Joback Method
cpg	65.29	J/mol×K	283.02	Joback Method
cpg	69.11	J/mol×K	310.42	Joback Method
cpg	72.61	J/mol×K	337.81	Joback Method
cpg	83.79	J/mol×K	447.40	Joback Method
cpl	163.80	J/mol×K	293.00	NIST Webbook
hvapt	17.80	kJ/mol	308.00	NIST Webbook
hvapt	17.70	kJ/mol	213.50	NIST Webbook
hvapt	19.10	kJ/mol	190.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.46449e+01
Coeff. B	-3.96443e+03
Coeff. C	-1.17615e+01
Coeff. D	3.40177e-05
Temperature range (K), min.	105.15
Temperature range (K), max.	340.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1502.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75638&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1502
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
ea:	Electron affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
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
rhoc:	Critical density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume