bromotrifluoroethylene

Other names:	TRIFLUOROBROMOETHYLENE
	TRIFLUOROVINYL BROMIDE
Inchi:	InChI=1S/C2BrF3/c3-1(4)2(5)6
InchiKey:	AYCANDRGVPTASA-UHFFFAOYSA-N
Formula:	C2BrF3
SMILES:	FC(F)=C(F)Br
Mol. weight [g/mol]:	160.92
CAS:	598-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-541.03	kJ/mol	Joback Method
hf	-548.97	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hvap	24.15	kJ/mol	Joback Method
ie	10.11	eV	NIST Webbook
ie	9.67	eV	NIST Webbook
log10ws	-2.49		Crippen Method
logp	2.416		Crippen Method
mcvol	57.550	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
tb	272.00 ± 1.00	K	NIST Webbook
tc	484.11	K	Joback Method
tf	140.87	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	78.58	J/mol×K	313.05	Joback Method
cpg	82.33	J/mol×K	341.56	Joback Method
cpg	85.79	J/mol×K	370.07	Joback Method
cpg	88.99	J/mol×K	398.58	Joback Method
cpg	91.92	J/mol×K	427.09	Joback Method

cpg	94.62	J/mol×K	455.60	Joback Method
cpg	97.09	J/mol×K	484.11	Joback Method
hvapt	25.00	kJ/mol	300.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1712.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598732&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume