Bromochlorodifluoromethane

Other names:	BCF
	CF2BrCl
	Chlorobromodifluoromethane
	Chlorodifluorobromomethane
	Chlorodifluoromonobromomethane
	Daiflon 12B1
	Difluorochlorobromomethane
	Flugex 12B1
	Fluorocarbon 1211
	Freon 12B1
	Halon 1211
	Methane, bromochlorodifluoro-
	R 12 B1
	UN 1974
Inchi:	InChI=1S/CBrClF2/c2-1(3,4)5
InchiKey:	MEXUFEQDCXZEON-UHFFFAOYSA-N
Formula:	CBrClF2
SMILES:	FC(F)(Cl)Br
Mol. weight [g/mol]:	165.37
CAS:	353-59-3

Physical Properties

Property code	Value	Unit	Source
gf	-426.85	kJ/mol	Joback Method
hf	-454.35	kJ/mol	Joback Method
hfus	6.57	kJ/mol	Joback Method
hvap	25.71	kJ/mol	Joback Method
ie	11.83	eV	NIST Webbook
ie	11.21 ± 0.02	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	2.170		Crippen Method
mcvol	58.230	ml/mol	McGowan Method
pc	5462.66	kPa	Joback Method
rinpol	405.00		NIST Webbook
rinpol	398.00		NIST Webbook
rinpol	405.00		NIST Webbook
rinpol	398.00		NIST Webbook

tb	270.60	K	NIST Webbook
tc	508.13	K	Joback Method
tf	194.35	K	Joback Method
vc	0.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	75.41	J/mol×K	321.18	Joback Method
cpg	90.00	J/mol×K	476.97	Joback Method
cpg	87.74	J/mol×K	445.82	Joback Method
cpg	85.17	J/mol×K	414.66	Joback Method
cpg	82.28	J/mol×K	383.50	Joback Method
cpg	79.03	J/mol×K	352.34	Joback Method
cpg	91.97	J/mol×K	508.13	Joback Method
hvapt	18.70	kJ/mol	230.50	NIST Webbook
hvapt	26.00	kJ/mol	230.50	NIST Webbook
hvapt	23.10	kJ/mol	415.00	NIST Webbook
hvapt	22.40	kJ/mol	362.00	NIST Webbook
hvapt	23.10	kJ/mol	240.50	NIST Webbook
hvapt	23.00	kJ/mol	296.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.14922e+01
Coeff. B	-4.38507e+03
Coeff. C	-7.38664e+00
Coeff. D	1.03430e-05
Temperature range (K), min.	114.00
Temperature range (K), max.	426.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1500.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C353593&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1500
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume