

Methane, bromochlorofluoro-

Other names:	Bromochlorofluoromethane Fluorochlorobromomethane
Inchi:	InChI=1S/CHBrClF/c2-1(3)4/h1H
InchiKey:	YNKZSBSRKWVMEZ-UHFFFAOYSA-N
Formula:	CHBrClF
SMILES:	FC(Cl)Br
Mol. weight [g/mol]:	147.37
CAS:	593-98-6

Physical Properties

Property code	Value	Unit	Source
gf	-237.32	kJ/mol	Joback Method
hf	-254.77	kJ/mol	Joback Method
hfus	7.39	kJ/mol	Joback Method
hvap	27.44	kJ/mol	Joback Method
ie	10.98 ± 0.05	eV	NIST Webbook
ie	11.13 ± 0.06	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.873		Crippen Method
mcvol	56.460	ml/mol	McGowan Method
pc	5747.92	kPa	Joback Method
tb	324.70	K	Joback Method
tc	514.68	K	Joback Method
tf	176.34	K	Joback Method
vc	0.214	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	66.61	J/mol×K	324.70	Joback Method
cpg	69.20	J/mol×K	356.36	Joback Method
cpg	71.61	J/mol×K	388.03	Joback Method
cpg	73.85	J/mol×K	419.69	Joback Method
cpg	75.93	J/mol×K	451.36	Joback Method

cpg	77.86	J/mol×K	483.02	Joback Method
cpg	79.64	J/mol×K	514.68	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52639e+01
Coeff. B	-3.29108e+03
Temperature range (K), min.	219.75
Temperature range (K), max.	330.68

Sources

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
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=C593986&Units=SI

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
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

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

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