Halothane

Other names:	(.+/-.))-Halothane
	1,1,1-Trifluoro-2-bromo-2-chloroethane
	1,1,1-Trifluoro-2-chloro-2-bromoethane
	1-Bromo-1-chloro-2,2,2-trifluoroethane
	2,2,2-Trifluoro-1-chloro-1-bromoethane
	2-Bromo-2-chloro-1,1,1-trifluoroethane
	Alotano
	Anestan
	Bromochlorotrifluoroethane
	CF3CHClBr
	Chalothane
	Ethane, 1-bromo-1-chloro-2,2,2-trifluoro-
	Ethane, 2-bromo-2-chloro-1,1,1-trifluoro-
	FREON 123B1
	Fluktan
	Fluorotane
	Fluorothane
	Fluothane
	Ftorotan
	Ftuorotan
	Halan
	Halotan
	Halotano
	Halothan
	Halsan
	NSC 143490
	Narcotan
	Narcotane
	Narcotann ne-spofa
	Narkotan
	Rhodialothan
Inchi:	InChI=1S/C2HBrClF3/c3-1(4)2(5,6)7/h1H
InchiKey:	BCQZXOMGPXTTIC-UHFFFAOYSA-N
Formula:	C2HBrClF3
SMILES:	FC(F)(F)C(Cl)Br
Mol. weight [g/mol]:	197.38
CAS:	151-67-7

Physical Properties

Property code	Value	Unit	Source
chl	-761.60 ± 3.20	kJ/mol	NIST Webbook
gf	-615.68	kJ/mol	Joback Method
hf	-699.90 ± 3.80	kJ/mol	NIST Webbook
hfl	-720.00 ± 4.90	kJ/mol	NIST Webbook
hfus	8.72	kJ/mol	Joback Method
hvap	29.80	kJ/mol	NIST Webbook
hvap	29.80 ± 0.40	kJ/mol	NIST Webbook
hvap	29.56 ± 0.33	kJ/mol	NIST Webbook
hvap	29.60 ± 0.30	kJ/mol	NIST Webbook
hvap	29.60 ± 0.10	kJ/mol	NIST Webbook
ie	11.00	eV	NIST Webbook
ie	11.20	eV	NIST Webbook
log10ws	-1.53		Aqueous Solubility Prediction Method
log10ws	-1.71		Estimated Solubility Method
logp	2.509		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	555.00		NIST Webbook
rinpol	541.00		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	543.00		NIST Webbook
ripol	858.00		NIST Webbook
tb	323.40	K	NIST Webbook
tb	596.40 ± 0.40	K	NIST Webbook
tb	323.00	K	NIST Webbook
tb	323.30	K	NIST Webbook
tb	323.42 ± 0.01	K	NIST Webbook
tc	496.30	K	NIST Webbook
tf	157.40 ± 0.20	K	NIST Webbook
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.51	J/mol×K	523.53	Joback Method
cpg	117.35	J/mol×K	373.00	Joback Method
cpg	122.16	J/mol×K	403.10	Joback Method
cpg	126.55	J/mol×K	433.21	Joback Method
cpg	130.56	J/mol×K	463.31	Joback Method
cpg	134.21	J/mol×K	493.42	Joback Method
cpg	112.10	J/mol×K	342.89	Joback Method
cpl	156.60	J/mol×K	298.15	NIST Webbook
hfust	4.84	kJ/mol	154.70	NIST Webbook
hfust	4.84	kJ/mol	157.40	NIST Webbook
hfust	4.84	kJ/mol	154.70	NIST Webbook
hvapt	28.08	kJ/mol	323.30	NIST Webbook
hvapt	30.00	kJ/mol	310.50	NIST Webbook
hvapt	33.20	kJ/mol	275.50	NIST Webbook
hvapt	28.70 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	27.80 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	26.80 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	34.30	kJ/mol	272.50	NIST Webbook
sfust	30.70	J/mol×K	157.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30696e+01
Coeff. B	-2.19144e+03
Coeff. C	-6.40470e+01
Temperature range (K), min.	223.15
Temperature range (K), max.	346.52

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	1.11666e+02
Coeff. B	-7.03230e+03
Coeff. C	-1.51373e+01
Coeff. D	2.08113e-05
Temperature range (K), min.	222.00
Temperature range (K), max.	328.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Interactions of volatile organic compounds with the ionic liquid 1-ethyl-3-methylimidazolium tetracyanoborate:	https://www.doi.org/10.1016/j.jct.2011.09.028
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1548
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1548
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Interactions of volatile organic compounds with the ionic liquids 1-butyl-1-methylpyrrolidinium tetracyanoborate and 1-butyl-1-methylpyrrolidinium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2012.09.017
Interactions of Volatile Organic Compounds with the Ionic Liquid 1-Butyl-1-methylpyrrolidinium Tricyanomethanide:	https://www.doi.org/10.1021/je200822w
Infinite dilution activity coefficients of volatile organic compounds in two ionic liquids composed of the tris(pentafluoroethyl) trifluorophosphate [FAP] anion and a functionalized cation:	https://www.doi.org/10.1016/j.jct.2013.05.035
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-Methyl-3-methylimidazolium methanesulfonate:	https://www.doi.org/10.1016/j.fluid.2010.10.008
NIST:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C151677&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1548
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume