

ETHANE, 2-BROMO-2-CHLORO-1,1,1-TRIFLUORO-

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 CF ₃ CHClBr Chalothane Ethane, 1-bromo-1-chloro-2,2,2-trifluoro- Fluktan Fluorotane Fluorothane Ftorotan Ftuorotan Halan Halotan Halotano Halothan Halsan NSC 143490 Narcotan Narcotane Narcotann ne-spofo Narkotan Rhodialothan fluothane freon 123B1 halothane
Inchi:	InChI=1S/C2HBrClF3/c3-1(4)2(5,6)7/h1H
InchiKey:	BCQZXOMGPXTTIC-UHFFFAOYSA-N
Formula:	C ₂ HBrClF ₃
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
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	-1.71		Estimated Solubility Method
log10ws	-1.53		Aqueous Solubility Prediction Method
logp	2.509		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	533.00		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	555.00		NIST Webbook
rinpol	541.00		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	543.00		NIST Webbook
ripol	858.00		NIST Webbook
tb	323.00	K	NIST Webbook
tb	323.42 ± 0.01	K	NIST Webbook
tb	596.40 ± 0.40	K	NIST Webbook
tb	323.30	K	NIST Webbook
tb	323.40	K	NIST Webbook
tc	496.30	K	NIST Webbook
tf	157.40 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

Sources

KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1548
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1548
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-butyl-3-methylimidazolium methanesulfonate:	https://www.doi.org/10.1016/j.fluid.2010.10.008
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/ci990307l
Interactions of Volatile Organic Compounds with the Ionic Liquid 1-butyl-3-methylpyrrolidinium Dicyanamide:	https://www.doi.org/10.1021/jc200822w
Interactions of volatile organic compounds with the ionic liquid 1-butyl-3-methylpyrrolidinium tetracyanoborate:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C151677&Units=SI
Estimate Solubility Method:	https://www.doi.org/10.1016/j.jct.2011.09.028
Joback Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
Interactions of volatile organic compounds with the ionic liquids 1-butyl-3-methylpyrrolidinium tetracyanoborate and 1-butyl-3-methylpyrrolidinium hexafluorophosphate:	http://link.springer.com/article/10.1007/BF02311772
Estimate Solubility Method:	https://www.doi.org/10.1016/j.jct.2012.09.017
Joback Method:	https://www.doi.org/10.1016/j.jct.2013.05.035
Interactions of volatile organic compounds with the ionic liquid 1-butyl-3-methylpyrrolidinium hexafluorophosphate:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
vpap:	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

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