

Ethane, 1-bromo-2-chloro-1,1,2-trifluoro-

Other names:	1,1,2-Trifluoro-1-bromo-2-chloroethane 1-bromo-2-chloro-1,1,2-trifluoroethane
Inchi:	InChI=1S/C2HBrClF3/c3-2(6,7)1(4)5/h1H
InchiKey:	KFTODZKBBUMDQB-UHFFFAOYSA-N
Formula:	C2HBrClF3
SMILES:	FC(Cl)C(F)(F)Br
Mol. weight [g/mol]:	197.38
CAS:	354-06-3

Physical Properties

Property code	Value	Unit	Source
chl	-806.30 ± 5.20	kJ/mol	NIST Webbook
hf	-654.70 ± 5.60	kJ/mol	NIST Webbook
hfl	-675.30 ± 6.40	kJ/mol	NIST Webbook
hfus	8.72	kJ/mol	Joback Method
hvap	30.00 ± 0.10	kJ/mol	NIST Webbook
hvap	30.50	kJ/mol	NIST Webbook
hvap	30.12	kJ/mol	NIST Webbook
ie	11.46	eV	Cheméo Relay (1.0)
log10ws	-2.26		Cheméo Relay (1.0)
logp	2.509		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
tb	325.50 ± 2.50	K	NIST Webbook
tb	325.60	K	NIST Webbook
tc	499.80	K	NIST Webbook
tf	146.20 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.16	J/mol×K	403.10	Joback Method
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	112.10	J/mol×K	342.89	Joback Method
cpg	117.35	J/mol×K	373.00	Joback Method
cpl	160.30	J/mol×K	298.15	NIST Webbook
hfust	4.38	kJ/mol	146.20	NIST Webbook
hfust	4.38	kJ/mol	146.20	NIST Webbook
hfust	4.38	kJ/mol	146.20	NIST Webbook
hvapt	27.20 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	28.10 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	29.00 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	28.31	kJ/mol	325.60	NIST Webbook
sfust	29.90	J/mol×K	146.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34672e+01
Coeff. B	-2.34327e+03
Coeff. C	-6.08390e+01
Temperature range (K), min.	238.63
Temperature range (K), max.	348.16

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C354063&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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
pvap:	Vapor pressure
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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