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

Other names:	2,2,2-Trifluoroethyl bromide
	2-bromo-1,1,1-trifluoroethane
	«beta» «beta» «beta»-Trifluoroethyl bromide
Inchi:	InChI=1S/C2H2BrF3/c3-1-2(4,5)6/h1H2
InchiKey:	TZNJHEHAYZJBHR-UHFFFAOYSA-N
Formula:	C2H2BrF3
SMILES:	FC(F)(F)CBr
Mol. weight [g/mol]:	162.94
CAS:	421-06-7

Physical Properties

Property code	Value	Unit	Source
hf	-695.00 ± 2.00	kJ/mol	NIST Webbook
hfus	8.05	kJ/mol	Joback Method
ie	11.31	eV	Cheméo Relay (1.0)
logp	1.944		Crippen Method
mcvol	61.850	ml/mol	McGowan Method
pc	4710.65	kPa	Joback Method
tb	299.00	K	NIST Webbook
tb	299.20	K	NIST Webbook
tb	248.00 ± 3.00	K	NIST Webbook
tc	458.55	K	Cheméo Relay (1.0)
tf	166.16	K	Cheméo Relay (1.0)
vc	0.231	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.90	J/mol×K	305.90	Joback Method
cpg	97.25	J/mol×K	333.54	Joback Method
cpg	102.22	J/mol×K	361.18	Joback Method
cpg	106.85	J/mol×K	388.82	Joback Method
cpg	111.14	J/mol×K	416.46	Joback Method
cpg	115.11	J/mol×K	444.09	Joback Method

cpg	118.78	J/mol×K	471.73	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50964e+01
Coeff. B	-3.13451e+03
Temperature range (K), min.	211.67
Temperature range (K), max.	320.66

Sources

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):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C421067&Units=SI

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
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