

2-Bromo-1,1,1-trifluoroethane

Other names:	2,2,2-Trifluoroethyl bromide Ethane, 2-bromo-1,1,1-trifluoro- «beta» «beta» «beta»-Trifluoroethyl bromide Â«betaÂ» Â«betaÂ» Â«betaÂ»-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
gf	-601.31	kJ/mol	Joback Method
hf	-695.00 ± 2.00	kJ/mol	NIST Webbook
hfus	8.05	kJ/mol	Joback Method
hvap	22.73	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
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	471.73	K	Joback Method
tf	176.29	K	Joback Method
vc	0.253	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.90	J/molxK	305.90	Joback Method
cpg	97.25	J/molxK	333.54	Joback Method
cpg	102.22	J/molxK	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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50964e+01
Coeff. B	-3.13451e+03
Temperature range (K), min.	211.67
Temperature range (K), max.	320.66

Sources

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

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
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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