

Methane, tribromofluoro-

Other names:	CFBr3 Fluorotribromomethane Tribromofluoromethane
Inchi:	InChI=1S/CBr3F/c2-1(3,4)5
InchiKey:	IHZAEIHJPNTART-UHFFFAOYSA-N
Formula:	CBr3F
SMILES:	FC(Br)(Br)Br
Mol. weight [g/mol]:	270.72
CAS:	353-54-8

Physical Properties

Property code	Value	Unit	Source
gf	-191.47	kJ/mol	Joback Method
hf	-189.84	kJ/mol	Joback Method
hfus	9.87	kJ/mol	Joback Method
hvap	35.01	kJ/mol	Joback Method
ie	10.67 ± 0.01	eV	NIST Webbook
ie	10.67 ± 0.01	eV	NIST Webbook
log10ws	-2.99		Crippen Method
logp	2.752		Crippen Method
mcvol	79.220	ml/mol	McGowan Method
pc	7790.05	kPa	Joback Method
tb	379.50 ± 0.50	K	NIST Webbook
tc	654.98	K	Joback Method
tf	283.44	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.31	J/molxK	416.80	Joback Method
cpg	95.34	J/molxK	456.50	Joback Method
cpg	97.78	J/molxK	496.19	Joback Method
cpg	99.70	J/molxK	535.89	Joback Method

cpg	101.17	J/mol×K	575.59	Joback Method
cpg	102.26	J/mol×K	615.29	Joback Method
cpg	103.03	J/mol×K	654.98	Joback Method
hvapt	34.40	kJ/mol	347.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54772e+01
Coeff. B	-4.12255e+03
Temperature range (K), min.	271.41
Temperature range (K), max.	405.54

Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

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

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C353548&Units=SI>

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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