Methyl fluoride

Other names:	CH3F
	FREON 41
	Fluoromethane
	HFC-41
	Methane, fluoro-
	R 41
	R-41
	REFRIGERANT-41
	Refrigerant gas R 41
	UN 2454
Inchi:	InChI=1S/CH3F/c1-2/h1H3
InchiKey:	NBVXSUQYWXRMNV-UHFFFAOYSA-N
Formula:	CH3F
SMILES:	CF
Mol. weight [g/mol]:	34.03
CAS:	593-53-3

Physical Properties

Property code	Value	Unit	Source
af	0.1870		KDB
affp	598.90	kJ/mol	NIST Webbook
basg	571.50	kJ/mol	NIST Webbook
dm	1.80	debye	KDB
gf	-210.10	kJ/mol	KDB
hf	-247.00	kJ/mol	NIST Webbook
hf	-234.00	kJ/mol	KDB
hfus	1.43	kJ/mol	Joback Method
hvap	17.00	kJ/mol	Joback Method
ie	12.50	eV	NIST Webbook
ie	12.54	eV	NIST Webbook
ie	13.05	eV	NIST Webbook
ie	13.05	eV	NIST Webbook
ie	13.04	eV	NIST Webbook
ie	12.50 ± 0.04	eV	NIST Webbook
ie	12.45	eV	NIST Webbook
ie	12.54	eV	NIST Webbook
log10ws	-0.09		Crippen Method

logp	0.586		Crippen Method
mcvol	26.720	ml/mol	McGowan Method
pc	5870.00 ± 58.65	kPa	NIST Webbook
pc	5880.00	kPa	KDB
pc	5876.85 ± 20.26	kPa	NIST Webbook
pt	0.37 ± 0.01	kPa	NIST Webbook
rhoc	313.10 ± 2.04	kg/m3	NIST Webbook
rhoc	312.08 ± 2.04	kg/m3	NIST Webbook
rhoc	311.06 ± 0.31	kg/m3	NIST Webbook
rhoc	300.31 ± 0.31	kg/m3	NIST Webbook
rinpol	173.00		NIST Webbook
rinpol	217.00		NIST Webbook
rinpol	173.00		NIST Webbook
tb	194.60	K	NIST Webbook
tb	194.74	K	KDB
tb	195.00 ± 2.00	K	NIST Webbook
tb	195.00 ± 2.00	K	NIST Webbook
tc	317.70 ± 0.05	K	NIST Webbook
tc	317.40 ± 0.50	K	NIST Webbook
tc	317.80	K	KDB
tf	131.30	K	KDB
vc	0.113	m3/kmol	KDB
zc	0.2514580		KDB
zra	0.25		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	42.46	J/mol×K	364.58	Joback Method
cpg	32.48	J/mol×K	245.39	Joback Method
cpg	34.57	J/mol×K	269.23	Joback Method
cpg	36.61	J/mol×K	293.07	Joback Method
cpg	38.61	J/mol×K	316.90	Joback Method
cpg	40.56	J/mol×K	340.74	Joback Method
cpg	30.34	J/mol×K	221.55	Joback Method
hvapt	17.90	kJ/mol	172.00	NIST Webbook
hvapt	16.90	kJ/mol	223.50	NIST Webbook
hvapt	16.90	kJ/mol	264.00	NIST Webbook
hvapt	17.10	kJ/mol	174.50	NIST Webbook
hvapt	16.40	kJ/mol	191.00	NIST Webbook
hvapt	17.70	kJ/mol	183.50	NIST Webbook

rhol	843.00	kg/m3	213.00	KDB
virco2	-1.96e-04	m3/mol	303.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System
virco2	-1.98e-04	m3/mol	303.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System
virco2	-1.82e-04	m3/mol	313.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System
virco2	-1.69e-04	m3/mol	323.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System
virco2	-1.70e-04	m3/mol	323.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System
virco2	-1.58e-04	m3/mol	333.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System
virco2	-1.57e-04	m3/mol	333.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System
virco2	-1.46e-04	m3/mol	343.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System

virco2	-1.45e-04	m3/mol	343.15	Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44665e+01
Coeff. B	-1.73654e+03
Coeff. C	-1.86690e+01
Temperature range (K), min.	131.35
Temperature range (K), max.	317.28

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.72038e+01
Coeff. B	-3.40443e+03
Coeff. C	-8.74270e+00
Coeff. D	2.55698e-05
Temperature range (K), min.	131.35
Temperature range (K), max.	317.70

Datasets

Amount density, mol/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Amount density, mol/m3 - Liquid
298.15	10000.00	18682.0
298.15	20000.00	20053.0
298.15	30000.00	21083.0

298.15	40000.00	21759.0
298.15	50000.00	22486.0
298.15	75000.00	23844.0
298.15	100000.00	25081.0
298.15	125000.00	26115.0
298.15	150000.00	26939.0
298.15	175000.00	27613.0
298.15	200000.00	28461.0
298.15	225000.00	29075.0
298.15	250000.00	29602.0
323.15	10000.00	15293.0
323.15	20000.00	18173.0
323.15	30000.00	19545.0
323.15	40000.00	20471.0
323.15	50000.00	21223.0
323.15	75000.00	22881.0
323.15	100000.00	24120.0
323.15	125000.00	25197.0
323.15	150000.00	26148.0
323.15	175000.00	26906.0
323.15	200000.00	27693.0
323.15	225000.00	28354.0
323.15	250000.00	29065.0
348.15	10000.00	9022.0
348.15	20000.00	15768.0
348.15	30000.00	17784.0
348.15	40000.00	19055.0
348.15	50000.00	19941.0
348.15	75000.00	21862.0
348.15	100000.00	23127.0
348.15	125000.00	24249.0
348.15	150000.00	25228.0
348.15	175000.00	26075.0
348.15	200000.00	26861.0
348.15	225000.00	27676.0
348.15	250000.00	28326.0
348.15	275000.00	28854.0
373.15	10000.00	5593.0
373.15	20000.00	13203.0
373.15	30000.00	15941.0
373.15	40000.00	17522.0
373.15	50000.00	18608.0
373.15	75000.00	20679.0
373.15	100000.00	22169.0

373.15	125000.00	23420.0
373.15	150000.00	24421.0
373.15	175000.00	25343.0
373.15	200000.00	26177.0
373.15	225000.00	26940.0
373.15	250000.00	27658.0
373.15	275000.00	28315.0
373.15	300000.00	28877.0
398.15	10000.00	4369.0
398.15	20000.00	10762.0
398.15	30000.00	14185.0
398.15	40000.00	16132.0
398.15	50000.00	17459.0
398.15	75000.00	19701.0
398.15	100000.00	21286.0
398.15	125000.00	22606.0
398.15	150000.00	23648.0
398.15	175000.00	24633.0
398.15	200000.00	25482.0
398.15	225000.00	26356.0
398.15	250000.00	27118.0
398.15	275000.00	27802.0
398.15	300000.00	28484.0
423.15	10000.00	3730.0
423.15	20000.00	8871.0
423.15	30000.00	12585.0
423.15	40000.00	14667.0
423.15	50000.00	16196.0
423.15	75000.00	18629.0
423.15	100000.00	20311.0
423.15	125000.00	21652.0
423.15	150000.00	22817.0
423.15	175000.00	23915.0
423.15	200000.00	24809.0
423.15	225000.00	25729.0
423.15	250000.00	26561.0
423.15	275000.00	27320.0
423.15	300000.00	28100.0
448.15	10000.00	3301.0
448.15	20000.00	7575.0
448.15	30000.00	11085.0
448.15	40000.00	13389.0
448.15	50000.00	15132.0
448.15	75000.00	17710.0

448.15	100000.00	19553.0
448.15	125000.00	20921.0
448.15	150000.00	22148.0
448.15	175000.00	23215.0
448.15	200000.00	24204.0
448.15	225000.00	25117.0
448.15	250000.00	25987.0
448.15	275000.00	26809.0
448.15	300000.00	27602.0
473.15	10000.00	2985.0
473.15	20000.00	6589.0
473.15	30000.00	9889.0
473.15	40000.00	12343.0
473.15	50000.00	13991.0
473.15	75000.00	16875.0
473.15	100000.00	18794.0
473.15	125000.00	20232.0
473.15	150000.00	21460.0
473.15	175000.00	22541.0
473.15	200000.00	23578.0
473.15	225000.00	24571.0
473.15	250000.00	25446.0
473.15	275000.00	26314.0
473.15	300000.00	27154.0
523.15	10000.00	2531.0
523.15	20000.00	5317.0
523.15	30000.00	8109.0
523.15	40000.00	10474.0
523.15	50000.00	12159.0
523.15	75000.00	15456.0
523.15	100000.00	17485.0
523.15	125000.00	19044.0
523.15	150000.00	20280.0
523.15	175000.00	21353.0
523.15	200000.00	22496.0
523.15	225000.00	23496.0
523.15	250000.00	24385.0
523.15	275000.00	25280.0
523.15	300000.00	26290.0
573.15	10000.00	2218.0
573.15	20000.00	4525.0
573.15	30000.00	6937.0
573.15	40000.00	9023.0
573.15	50000.00	10721.0

573.15	75000.00	14186.0
573.15	100000.00	16345.0
573.15	125000.00	17915.0
573.15	150000.00	19276.0
573.15	175000.00	20371.0
573.15	200000.00	21514.0
573.15	225000.00	22632.0
573.15	250000.00	23465.0
573.15	275000.00	24391.0
573.15	300000.00	25343.0

Reference *https://www.doi.org/10.1016/j.jct.2007.01.003*

Sources

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Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of hydrofluorocarbons in aromatic solvents and alcohols:	https://www.doi.org/10.1016/j.fluid.2012.09.013
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solubility of HFCs in lower alcohols:	https://www.doi.org/10.1016/j.fluid.2011.01.003
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1531.mol
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Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
PVTx Measurements for the R116 + CO2 and R41 + CO2 Systems. New Isochoric Apparatus:	https://www.doi.org/10.1021/je049939g
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NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C593533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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Solubility of Hydrofluorocarbons in Halobenzene Solvents:	https://www.doi.org/10.1021/je500525q
Virial Coefficients from Burnett Measurements for the Carbon Dioxide + Fluoromethane System:	https://www.doi.org/10.1021/je025630q

Legend

af:	Acentric Factor

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
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
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rhoml:	Liquid Amount Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
virco2:	2nd virial coefficient
zc:	Critical Compressibility
zra:	Rackett Parameter