

Propane, 1,1,1-trifluoro-

Other names:	1,1,1-trifluoropropane CH ₃ CH ₂ CF ₃
Inchi:	InChI=1S/C3H5F3/c1-2-3(4,5)6/h2H2,1H3
InchiKey:	KDWQLICBSFIDRM-UHFFFAOYSA-N
Formula:	C ₃ H ₅ F ₃
SMILES:	CCC(F)(F)F
Mol. weight [g/mol]:	98.07
CAS:	421-07-8

Physical Properties

Property code	Value	Unit	Source
gf	-607.21	kJ/mol	Joback Method
hf	-702.33	kJ/mol	Joback Method
hfus	5.35	kJ/mol	Joback Method
hvap	18.53	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.959		Crippen Method
mvol	58.440	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	361.00		NIST Webbook
tb	262.62	K	Joback Method
tc	404.58	K	Joback Method
tf	127.76	K	Joback Method
vc	0.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.34	J/mol×K	262.62	Joback Method
cpg	95.91	J/mol×K	286.28	Joback Method
cpg	102.19	J/mol×K	309.94	Joback Method
cpg	108.18	J/mol×K	333.60	Joback Method
cpg	113.90	J/mol×K	357.26	Joback Method
cpg	119.35	J/mol×K	380.92	Joback Method

cpg

124.53

J/mol×K

404.58

Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41003e+01
Coeff. B	-2.16710e+03
Coeff. C	-3.26000e+01
Temperature range (K), min.	189.49
Temperature range (K), max.	279.18

Sources

Joback Method:

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

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C421078&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/ci9903071>

Crippen Method:

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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices

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

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