(Trifluoromethyl)acetylene

Other names:	1,1,1-Trifluoropropyne
	1-Propyne, 3,3,3-trifluoro-
	3,3,3-Trifluoro-1-propyne
	3,3,3-Trifluoropropyne
	CF3C«equiv»CH
	CF3CÂ«equivÂ»CH
	Propyne, 3,3,3-trifluoro-
Inchi:	InChI=1S/C3HF3/c1-2-3(4,5)6/h1H
InchiKey:	PRDFNJUWGIQQBW-UHFFFAOYSA-N
Formula:	C3HF3
SMILES:	C#CC(F)(F)F
Mol. weight [g/mol]:	94.04
CAS:	661-54-1

Physical Properties

Property code	Value	Unit	Source
gf	-384.14	kJ/mol	Joback Method
hf	-410.43	kJ/mol	Joback Method
hfus	8.33	kJ/mol	Joback Method
hvap	18.38	kJ/mol	Joback Method
ie	11.96 ± 0.02	eV	NIST Webbook
ie	11.83	eV	NIST Webbook
log10ws	-1.54		Crippen Method
logp	1.182		Crippen Method
mcvol	49.840	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
tb	252.74	K	Joback Method
tc	404.30	K	Joback Method
tf	174.73	K	Joback Method
vc	0.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	77.10	J/mol×K	252.74	Joback Method
cpg	82.02	J/mol×K	278.00	Joback Method
cpg	86.63	J/mol×K	303.26	Joback Method
cpg	90.93	J/mol×K	328.52	Joback Method
cpg	94.95	J/mol×K	353.78	Joback Method
cpg	98.69	J/mol×K	379.04	Joback Method
cpg	102.16	J/mol×K	404.30	Joback Method
hvapt	21.50	kJ/mol	175.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	225.00	K	94.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57334e+01
Coeff. B	-2.52312e+03
Temperature range (K), min.	163.35
Temperature range (K), max.	242.10

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C661541&Units=SI

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume