1-Propyne, 3-chloro-

Other names:	2-Propynyl chloride
	3-Chloro-1-propyne
	3-Chloropropyne
	CH2ClC«equiv»CH
	CH2ClCÂ«equivÂ»CH
	Propargyl chloride
	Propyne, 3-chloro-
Inchi:	InChI=1S/C3H3Cl/c1-2-3-4/h1H,3H2
InchiKey:	LJZPPWWHKPGCHS-UHFFFAOYSA-N
Formula:	C3H3Cl
SMILES:	C#CCCl
Mol. weight [g/mol]:	74.51
CAS:	624-65-7

Physical Properties

Property code	Value	Unit	Source
gf	185.52	kJ/mol	Joback Method
hf	170.91	kJ/mol	Joback Method
hfus	10.70	kJ/mol	Joback Method
hvap	26.52	kJ/mol	Joback Method
ie	10.68	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
ie	10.76	eV	NIST Webbook
ie	10.76	eV	NIST Webbook
ie	10.76	eV	NIST Webbook
log10ws	-1.03		Crippen Method
logp	0.858		Crippen Method
mcvol	56.770	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
rinpol	545.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	545.00		NIST Webbook
rinpol	542.00		NIST Webbook
tb	330.00 ± 2.00	K	NIST Webbook
tb	331.20	K	NIST Webbook
tb	331.00	K	NIST Webbook
tc	480.05	K	Joback Method

tf	200.46	K	Joback Method
vc	0.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.18	J/mol×K	295.59	Joback Method
cpg	77.87	J/mol×K	326.33	Joback Method
cpg	81.36	J/mol×K	357.08	Joback Method
cpg	84.66	J/mol×K	387.82	Joback Method
cpg	87.78	J/mol×K	418.57	Joback Method
cpg	90.72	J/mol×K	449.31	Joback Method
cpg	93.51	J/mol×K	480.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41675e+01
Coeff. B	-2.83387e+03
Coeff. C	-3.42350e+01
Temperature range (K), min.	238.41
Temperature range (K), max.	354.23

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624657&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

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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