

2-Butyne, 1-chloro-

Other names:	1-Chloro-2-butyne
Inchi:	InChI=1S/C4H5Cl/c1-2-3-4-5/h4H2,1H3
InchiKey:	OKWUYBGGPXXFLS-UHFFFAOYSA-N
Formula:	C4H5Cl
SMILES:	CC#CCCl
Mol. weight [g/mol]:	88.54
CAS:	3355-17-7

Physical Properties

Property code	Value	Unit	Source
gf	173.67	kJ/mol	Joback Method
hf	130.67	kJ/mol	Joback Method
hfus	13.43	kJ/mol	Joback Method
hvap	31.04	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.249		Crippen Method
mcvol	70.860	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
rinpol	723.00		NIST Webbook
tb	337.35	K	Joback Method
tc	537.54	K	Joback Method
tf	270.86	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	97.99	J/mol×K	337.35	Joback Method
cpg	103.44	J/mol×K	370.71	Joback Method
cpg	108.69	J/mol×K	404.08	Joback Method
cpg	113.73	J/mol×K	437.44	Joback Method
cpg	118.57	J/mol×K	470.81	Joback Method
cpg	123.21	J/mol×K	504.17	Joback Method
cpg	127.67	J/mol×K	537.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56080e+01
Coeff. B	-3.61869e+03
Coeff. C	-4.57200e+01
Temperature range (K), min.	281.92
Temperature range (K), max.	398.69

Sources

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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=C3355177&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
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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