1-Butyne, 3-chloro-

Other names: 3-Chloro-1-butyne
3-chlorobut-1-yne
Inchi: InChI=1S/C4H5Cl/c1-3-4(2)5/h1,4H,2H3
InchiKey: PZFBULOUMNPBFA-UHFFFAOYSA-N
Formula: C4H5Cl
SMILES: C#CC(C)Cl
Mol. weight [g/mol]: 88.54
CAS: 21020-24-6

Physical Properties

Property code	Value	Unit	Source
gf	191.50	kJ/mol	Joback Method
hf	144.99	kJ/mol	Joback Method
hfus	9.76	kJ/mol	Joback Method
hvap	28.35	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.247		Crippen Method
mcvol	70.860	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	318.03	K	Joback Method
tc	508.03	K	Joback Method
tf	196.73	K	Joback Method
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.94	J/mol×K	318.03	Joback Method
cpg	106.68	J/mol×K	349.70	Joback Method
cpg	112.13	J/mol×K	381.36	Joback Method
cpg	117.30	J/mol×K	413.03	Joback Method
cpg	122.19	J/mol×K	444.69	Joback Method
cpg	126.83	J/mol×K	476.36	Joback Method
cpg	131.22	J/mol×K	508.03	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29558e+01
Coeff. B	-2.76409e+03
Coeff. C	-3.61290e+01
Temperature range (K), min.	254.32
Temperature range (K), max.	397.72

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=C21020246&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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