3-chloro-3-methyl-1-butyne

Inchi: InChI=1S/C5H7Cl/c1-4-5(2,3)6/h1H,2-3H3
InchiKey: QSILYWCNPOLKPN-UHFFFAOYSA-N
Formula: C5H7Cl
SMILES: C#CC(C)(C)Cl
Mol. weight [g/mol]: 102.56
CAS: 1111-97-3

Physical Properties

Property code	Value	Unit	Source
af	0.1622		Cheméo Relay (1.0)
gf	205.20	kJ/mol	Joback Method
hf	87.24	kJ/mol	Cheméo Relay (1.0)
hfus	8.46	kJ/mol	Joback Method
hvap	31.02	kJ/mol	Cheméo Relay (1.0)
ie	10.34	eV	Cheméo Relay (1.0)
log10ws	-2.00		Cheméo Relay (1.0)
logp	1.637		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	341.99	K	Cheméo Relay (1.0)
tc	524.11	K	Cheméo Relay (1.0)
tf	253.93	K	Cheméo Relay (1.0)
vc	0.300	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.35	J/mol×K	338.12	Joback Method
cpg	140.09	J/mol×K	371.24	Joback Method
cpg	148.23	J/mol×K	404.36	Joback Method
cpg	155.80	J/mol×K	437.48	Joback Method
cpg	162.84	J/mol×K	470.60	Joback Method
cpg	169.39	J/mol×K	503.72	Joback Method
cpg	175.46	J/mol×K	536.84	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.13940e+01
Coeff. B	-2.46679e+03
Coeff. C	-3.82140e+01
Temperature range (K), min.	260.32
Temperature range (K), max.	443.77

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

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