5-Chloro-1-pentyne

Other names: 1-Pentyne, 5-chloro-
5-chloropent-1-yne
Inchi: InChI=1S/C5H7Cl/c1-2-3-4-5-6/h1H,3-5H2
InchiKey: UXFIKVWAAMKFQE-UHFFFAOYSA-N
Formula: C5H7Cl
SMILES: C#CCCCCl
Mol. weight [g/mol]: 102.56
CAS: 14267-92-6

Physical Properties

Property code	Value	Unit	Source
gf	202.36	kJ/mol	Joback Method
hf	129.63	kJ/mol	Joback Method
hfus	15.88	kJ/mol	Joback Method
hvap	30.97	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.639		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
rinpol	735.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	732.00		NIST Webbook
rinpol	735.00		NIST Webbook
tb	341.15 ± 2.00	K	NIST Webbook
tb	386.00 ± 3.00	K	NIST Webbook
tb	387.00 ± 2.00	K	NIST Webbook
tc	526.60	K	Joback Method
tf	223.00	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.91	J/mol×K	341.35	Joback Method

cpg	138.07	J/mol×K	372.23	Joback Method
cpg	144.88	J/mol×K	403.10	Joback Method
cpg	151.37	J/mol×K	433.98	Joback Method
cpg	157.54	J/mol×K	464.85	Joback Method
cpg	163.40	J/mol×K	495.73	Joback Method
cpg	168.98	J/mol×K	526.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.00	K	19.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33739e+01
Coeff. B	-3.00867e+03
Coeff. C	-4.23700e+01
Temperature range (K), min.	272.28
Temperature range (K), max.	415.54

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14267926&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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