Pentane, 2-chloro-

Other names: 1-Methylbutyl chloride
2-Chloropentane
sec-Amyl chloride
Inchi: InChI=1S/C5H11Cl/c1-3-4-5(2)6/h5H,3-4H2,1-2H3
InchiKey: NFRKUDYZEVQXTE-UHFFFAOYSA-N
Formula: C5H11Cl
SMILES: CCCC(C)Cl
Mol. weight [g/mol]: 106.59
CAS: 625-29-6

Physical Properties

Property code	Value	Unit	Source
gf	-23.15	kJ/mol	Joback Method
hf	-167.55	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	36.02	kJ/mol	NIST Webbook
hvap	36.00	kJ/mol	NIST Webbook
log10ws	-2.63		Aqueous Solubility Prediction Method
logp	2.414		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	702.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	696.00		NIST Webbook
ripol	884.00		NIST Webbook
ripol	869.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	874.00		NIST Webbook
tb	369.75 ± 0.30	K	NIST Webbook
tb	368.65 ± 2.00	K	NIST Webbook
tb	370.01 ± 0.30	K	NIST Webbook
tb	369.85 ± 0.30	K	NIST Webbook
tc	527.49	K	Joback Method

tf	135.00 ± 4.00	K	NIST Webbook
tf	164.65	K	Aqueous Solubility Prediction Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.28	J/mol×K	380.24	Joback Method
cpg	169.22	J/mol×K	409.69	Joback Method
cpg	177.80	J/mol×K	439.14	Joback Method
cpg	201.54	J/mol×K	527.49	Joback Method
cpg	186.05	J/mol×K	468.59	Joback Method
cpg	193.96	J/mol×K	498.04	Joback Method
cpg	150.99	J/mol×K	350.79	Joback Method
dvisc	0.0003734	Pa×s	319.16	Joback Method
dvisc	0.0005253	Pa×s	287.54	Joback Method
dvisc	0.0008040	Pa×s	255.91	Joback Method
dvisc	0.0013876	Pa×s	224.28	Joback Method
dvisc	0.0028647	Pa×s	192.66	Joback Method
dvisc	0.0002823	Pa×s	350.79	Joback Method
dvisc	0.0078623	Pa×s	161.03	Joback Method
hvapt	31.90	kJ/mol	368.00	NIST Webbook
hvapt	33.50	kJ/mol	358.00	NIST Webbook
hvapt	35.20	kJ/mol	313.00	NIST Webbook
hvapt	36.20	kJ/mol	349.00	NIST Webbook
hvapt	34.40	kJ/mol	328.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42868e+01
Coeff. B	-3.11391e+03
Coeff. C	-4.65810e+01
Temperature range (K), min.	269.02
Temperature range (K), max.	393.52

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625296&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume