PENTANOYL CHLORIDE

Other names:	UN 2502
	Valeroyl chloride
	Valeryl chloride
	n-Valeroyl chloride
Inchi:	InChI=1S/C5H9ClO/c1-2-3-4-5(6)7/h2-4H2,1H3
InchiKey:	XGISHOFUAFNYQF-UHFFFAOYSA-N
Formula:	C5H9ClO
SMILES:	CCCCC(=O)Cl
Mol. weight [g/mol]:	120.58
CAS:	638-29-9

Physical Properties

Property code	Value	Unit	Source
af	0.3879		Cheméo Relay (1.0)
gf	-149.63	kJ/mol	Joback Method
hf	-298.86	kJ/mol	Cheméo Relay (1.0)
hfus	14.50	kJ/mol	Joback Method
hvap	34.64	kJ/mol	Cheméo Relay (1.0)
ie	10.29	eV	Cheméo Relay (1.0)
log10ws	-1.98		Cheméo Relay (1.0)
logp	1.942		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	809.40		NIST Webbook
tb	400.40 ± 0.60	K	NIST Webbook
tb	399.20	K	NIST Webbook
tc	571.80	K	Cheméo Relay (1.0)
tf	193.25	K	Cheméo Relay (1.0)
vc	0.348	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.83	J/mol×K	591.48	Joback Method

cpg	166.17	J/mol×K	405.10	Joback Method
cpg	182.77	J/mol×K	467.23	Joback Method
cpg	190.54	J/mol×K	498.29	Joback Method
cpg	197.97	J/mol×K	529.35	Joback Method
cpg	205.06	J/mol×K	560.42	Joback Method
cpg	174.65	J/mol×K	436.16	Joback Method
cpl	187.90	J/mol×K	298.00	NIST Webbook
dvisc	0.0008330	Pa×s	315.53	Joback Method
dvisc	0.0012390	Pa×s	285.67	Joback Method
dvisc	0.0037554	Pa×s	225.96	Joback Method
dvisc	0.0005998	Pa×s	345.39	Joback Method
dvisc	0.0004551	Pa×s	375.24	Joback Method
dvisc	0.0003596	Pa×s	405.10	Joback Method
dvisc	0.0020219	Pa×s	255.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66775e+01
Coeff. B	-4.93981e+03
Coeff. C	-1.25600e+01
Temperature range (K), min.	307.00
Temperature range (K), max.	447.17

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C638299&Units=SI

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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume