

1-Pentanol, 5-chloro-, acetate

Other names:	5-Chloro-n-amyl acetate 1-Acetoxy-5-chloropentane 5-Chloro-1-acetoxypentane 5-Chloro-1-amyl acetate 5-Chloro-1-pentanol acetate 5-Chloro-1-pentyl acetate 5-Chloropentyl acetate
Inchi:	InChI=1S/C7H13ClO2/c1-7(9)10-6-4-2-3-5-8/h2-6H2,1H3
InchiKey:	ZCYVIAZIVJNAMO-UHFFFAOYSA-N
Formula:	C7H13ClO2
SMILES:	CC(=O)OCCCCCl
Mol. weight [g/mol]:	164.63
CAS:	20395-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-237.79	kJ/mol	Joback Method
hf	-448.35	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.959		Crippen Method
mvol	129.170	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1142.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1143.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1652.00		NIST Webbook

ripol	1657.00		NIST Webbook
tb	473.28	K	Joback Method
tc	655.90	K	Joback Method
tf	270.73	K	Joback Method
vc	0.500	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.22	J/molxK	473.28	Joback Method
cpg	276.01	J/molxK	503.72	Joback Method
cpg	286.40	J/molxK	534.15	Joback Method
cpg	296.38	J/molxK	564.59	Joback Method
cpg	305.96	J/molxK	595.03	Joback Method
cpg	315.13	J/molxK	625.46	Joback Method
cpg	323.90	J/molxK	655.90	Joback Method
dvisc	0.0030645	Paxs	270.73	Joback Method
dvisc	0.0016518	Paxs	304.49	Joback Method
dvisc	0.0010072	Paxs	338.25	Joback Method
dvisc	0.0006719	Paxs	372.00	Joback Method
dvisc	0.0004794	Paxs	405.76	Joback Method
dvisc	0.0003603	Paxs	439.52	Joback Method
dvisc	0.0002820	Paxs	473.28	Joback Method

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=C20395282&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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