CHLOROACETIC ACID, PENTYL ESTER

Other names: 1-Pentanol, chloroacetate
Chloroacetic acid, pentyl ester
Pentyl chloroacetate
Inchi: InChI=1S/C7H13ClO2/c1-2-3-4-5-10-7(9)6-8/h2-6H2,1H3
InchiKey: SAOZOMQLKLWJAN-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCCCCOC(=O)CCl
Mol. weight [g/mol]: 164.63

Physical Properties

Property code	Value	Unit	Source
af	0.5363		Cheméo Relay (1.0)
hf	-533.10	kJ/mol	Cheméo Relay (1.0)
hfus	20.87	kJ/mol	Joback Method
hvap	47.75	kJ/mol	Cheméo Relay (1.0)
ie	10.13	eV	Cheméo Relay (1.0)
log10ws	-2.39		Cheméo Relay (1.0)
logp	1.959		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1089.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1100.20		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1106.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1609.00		NIST Webbook
tb	466.05	K	Cheméo Relay (1.0)
tc	652.32	K	Cheméo Relay (1.0)
tf	234.05	K	Cheméo Relay (1.0)
vc	0.480	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5411552&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
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