CHLOROMETHYL 5-CHLOROPENTANOATE

Other names: 5-Chloropentanoic acid, chloromethyl ester
Monochloromethyl 5-chloropentanoate
Inchi: InChI=1S/C6H10Cl2O2/c7-4-2-1-3-6(9)10-5-8/h1-5H2
InchiKey: VQDRONCNGCJOGI-UHFFFAOYSA-N
Formula: C6H10Cl2O2
SMILES: O=C(CCCCCl)OCCl
Mol. weight [g/mol]: 185.05

Physical Properties

Property code	Value	Unit	Source
hf	-530.23	kJ/mol	Cheméo Relay (1.0)
hfus	22.48	kJ/mol	Joback Method
hvap	58.38	kJ/mol	Cheméo Relay (1.0)
ie	10.30	eV	Cheméo Relay (1.0)
log10ws	-2.20		Cheméo Relay (1.0)
logp	2.135		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1227.00		NIST Webbook
ripol	1851.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1904.00		NIST Webbook
ripol	1851.00		NIST Webbook
tb	491.05	K	Cheméo Relay (1.0)
tc	687.49	K	Cheméo Relay (1.0)
tf	242.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.95	J/mol×K	487.83	Joback Method
cpg	258.21	J/mol×K	519.55	Joback Method
cpg	267.08	J/mol×K	551.28	Joback Method
cpg	275.57	J/mol×K	583.00	Joback Method
cpg	283.68	J/mol×K	614.72	Joback Method
cpg	291.42	J/mol×K	646.44	Joback Method
cpg	298.78	J/mol×K	678.17	Joback Method
dvisc	0.0028553	Pa×s	289.38	Joback Method
dvisc	0.0016272	Pa×s	322.45	Joback Method
dvisc	0.0010297	Pa×s	355.53	Joback Method
dvisc	0.0007043	Pa×s	388.61	Joback Method
dvisc	0.0005113	Pa×s	421.68	Joback Method
dvisc	0.0003889	Pa×s	454.75	Joback Method
dvisc	0.0003070	Pa×s	487.83	Joback Method

Sources

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=C80482355&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

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