5-chloropentyl chloroacetate

Other names: 1-Pentanol, 5-chloro, chloroacetate
Inchi: InChI=1S/C7H12Cl2O2/c8-4-2-1-3-5-11-7(10)6-9/h1-6H2
InchiKey: OWJFRQZEEQSFNQ-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: O=C(CCl)OCCCCCCl
Mol. weight [g/mol]: 199.07

Physical Properties

Property code	Value	Unit	Source
gf	-249.72	kJ/mol	Joback Method
hf	-464.09	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.178		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1346.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2138.00		NIST Webbook
tb	510.71	K	Joback Method
tc	698.85	K	Joback Method
tf	300.65	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.67	J/mol×K	510.71	Joback Method

cpg	301.04	J/mol×K	542.07	Joback Method
cpg	310.97	J/mol×K	573.42	Joback Method
cpg	320.46	J/mol×K	604.78	Joback Method
cpg	329.52	J/mol×K	636.14	Joback Method
cpg	338.15	J/mol×K	667.50	Joback Method
cpg	346.35	J/mol×K	698.85	Joback Method
dvisc	0.0028037	Pa×s	300.65	Joback Method
dvisc	0.0015651	Pa×s	335.66	Joback Method
dvisc	0.0009754	Pa×s	370.67	Joback Method
dvisc	0.0006596	Pa×s	405.68	Joback Method
dvisc	0.0004746	Pa×s	440.69	Joback Method
dvisc	0.0003585	Pa×s	475.70	Joback Method
dvisc	0.0002814	Pa×s	510.71	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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=R112466&Units=SI

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
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