

3-Chloropentanoic acid, chloromethyl ester

Other names:	Monochloromethyl 3-chloropentanoate
Inchi:	InChI=1S/C6H10Cl2O2/c1-2-5(8)3-6(9)10-4-7/h5H,2-4H2,1H3
InchiKey:	OJAHETHLCCYRJD-UHFFFAOYSA-N
Formula:	C6H10Cl2O2
SMILES:	CCC(Cl)CC(=O)OCCI
Mol. weight [g/mol]:	185.05

Physical Properties

Property code	Value	Unit	Source
gf	-260.58	kJ/mol	Joback Method
hf	-448.73	kJ/mol	Joback Method
hfus	18.95	kJ/mol	Joback Method
hvap	46.49	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.133		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1126.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1133.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1694.00		NIST Webbook
tb	487.39	K	Joback Method
tc	681.93	K	Joback Method
tf	274.38	K	Joback Method
vc	0.487	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.20	J/mol×K	487.39	Joback Method
cpg	258.74	J/mol×K	519.81	Joback Method
cpg	267.87	J/mol×K	552.24	Joback Method
cpg	276.59	J/mol×K	584.66	Joback Method
cpg	284.91	J/mol×K	617.08	Joback Method
cpg	292.82	J/mol×K	649.50	Joback Method
cpg	300.33	J/mol×K	681.93	Joback Method
dvisc	0.0038678	Paxs	274.38	Joback Method
dvisc	0.0019631	Paxs	309.88	Joback Method
dvisc	0.0011455	Paxs	345.38	Joback Method
dvisc	0.0007390	Paxs	380.88	Joback Method
dvisc	0.0005137	Paxs	416.39	Joback Method
dvisc	0.0003781	Paxs	451.89	Joback Method
dvisc	0.0002910	Paxs	487.39	Joback Method

Sources

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=U143760&Units=SI>

Crippen Method:

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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
ripol:	Polar retention indices

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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