CHLOROMETHYL 4-CHLOROPENTANOATE

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

Physical Properties

Property code	Value	Unit	Source
hf	-541.38	kJ/mol	Cheméo Relay (1.0)
hfus	18.95	kJ/mol	Joback Method
hvap	55.24	kJ/mol	Cheméo Relay (1.0)
logp	2.133		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
rinpol	1166.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1166.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1730.00		NIST Webbook
tb	480.66	K	Cheméo Relay (1.0)

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	Pa×s	274.38	Joback Method
dvisc	0.0019631	Pa×s	309.88	Joback Method
dvisc	0.0011455	Pa×s	345.38	Joback Method
dvisc	0.0007390	Pa×s	380.88	Joback Method
dvisc	0.0005137	Pa×s	416.39	Joback Method
dvisc	0.0003781	Pa×s	451.89	Joback Method
dvisc	0.0002910	Pa×s	487.39	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=C80418526&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
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature