CHLOROACETIC ACID, 3-CHLOROPROPYL ESTER

Other names: 1-Propanol, 3-chloro, chloroacetate
3-chloropropyl chloroacetate
Inchi: InChI=1S/C5H8Cl2O2/c6-2-1-3-9-5(8)4-7/h1-4H2
InchiKey: CWZVJVDIQWKNJX-UHFFFAOYSA-N
Formula: C5H8Cl2O2
SMILES: O=C(CCl)OCCCCl
Mol. weight [g/mol]: 171.02

Physical Properties

Property code	Value	Unit	Source
hf	-492.54	kJ/mol	Cheméo Relay (1.0)
hfus	19.89	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Cheméo Relay (1.0)
ie	10.47	eV	Cheméo Relay (1.0)
logp	1.397		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
rinpol	1138.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1134.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1851.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1909.00		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1909.00		NIST Webbook
tb	478.05	K	Cheméo Relay (1.0)
tc	680.00	K	Cheméo Relay (1.0)
tf	240.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.33	J/mol×K	464.95	Joback Method
cpg	217.34	J/mol×K	497.04	Joback Method
cpg	225.03	J/mol×K	529.12	Joback Method
cpg	232.40	J/mol×K	561.21	Joback Method
cpg	239.45	J/mol×K	593.30	Joback Method
cpg	246.19	J/mol×K	625.38	Joback Method
cpg	252.60	J/mol×K	657.47	Joback Method
dvisc	0.0028660	Pa×s	278.11	Joback Method
dvisc	0.0016697	Pa×s	309.25	Joback Method
dvisc	0.0010738	Pa×s	340.39	Joback Method
dvisc	0.0007436	Pa×s	371.53	Joback Method
dvisc	0.0005451	Pa×s	402.67	Joback Method
dvisc	0.0004178	Pa×s	433.81	Joback Method
dvisc	0.0003318	Pa×s	464.95	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62116556&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

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

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

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point