

CHLOROACETIC ACID, PROPYL ESTER

Other names:	Acetic acid, chloro-, propyl ester Propyl chloroacetate
Inchi:	InChI=1S/C5H9ClO2/c1-2-3-8-5(7)4-6/h2-4H2,1H3
InchiKey:	QJZNRCWAXUGABH-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	CCCOC(=O)CCl
Mol. weight [g/mol]:	136.58

Physical Properties

Property code	Value	Unit	Source
hf	-491.97	kJ/mol	Cheméo Relay (1.0)
hfus	15.69	kJ/mol	Joback Method
hvap	40.93	kJ/mol	Cheméo Relay (1.0)
ie	10.31	eV	Cheméo Relay (1.0)
log10ws	-1.35		Cheméo Relay (1.0)
logp	1.178		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	430.61	K	Cheméo Relay (1.0)
tc	610.23	K	Cheméo Relay (1.0)
tf	227.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.82	J/mol×K	427.52	Joback Method
cpg	195.11	J/mol×K	458.52	Joback Method
cpg	203.12	J/mol×K	489.53	Joback Method
cpg	210.84	J/mol×K	520.53	Joback Method
cpg	218.28	J/mol×K	551.53	Joback Method
cpg	225.43	J/mol×K	582.53	Joback Method
cpg	232.29	J/mol×K	613.54	Joback Method
dvisc	0.0029404	Pa×s	248.19	Joback Method
dvisc	0.0016595	Pa×s	278.08	Joback Method

dvisc	0.0010466	Pa×s	307.97	Joback Method
dvisc	0.0007162	Pa×s	337.86	Joback Method
dvisc	0.0005212	Pa×s	367.74	Joback Method
dvisc	0.0003979	Pa×s	397.63	Joback Method
dvisc	0.0003154	Pa×s	427.52	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=C5396247&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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