PROPIONIC ACID, 2-CHLORO-, PROPYL ESTER

Other names: Propanoic acid, 2-chloro, propyl ester
Propyl 2-chloropropanoate
Inchi: InChI=1S/C6H11ClO2/c1-3-4-9-6(8)5(2)7/h5H,3-4H2,1-2H3
InchiKey: XVDQGLUGZORASO-UHFFFAOYSA-N
Formula: C6H11ClO2
SMILES: CCCOC(=O)C(C)Cl
Mol. weight [g/mol]: 150.61

Physical Properties

Property code	Value	Unit	Source
hf	-531.39	kJ/mol	Cheméo Relay (1.0)
hfus	14.76	kJ/mol	Joback Method
hvap	45.09	kJ/mol	Cheméo Relay (1.0)
ie	10.37	eV	Cheméo Relay (1.0)
log10ws	-1.51		Cheméo Relay (1.0)
logp	1.567		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1327.00		NIST Webbook
tb	426.58	K	Cheméo Relay (1.0)

tc	604.99	K	Cheméo Relay (1.0)
tf	219.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.04	J/mol×K	449.96	Joback Method
cpg	234.96	J/mol×K	481.38	Joback Method
cpg	244.50	J/mol×K	512.81	Joback Method
cpg	253.66	J/mol×K	544.23	Joback Method
cpg	262.46	J/mol×K	575.65	Joback Method
cpg	270.88	J/mol×K	607.08	Joback Method
cpg	278.93	J/mol×K	638.50	Joback Method
dvisc	0.0043249	Pa×s	244.46	Joback Method
dvisc	0.0020836	Pa×s	278.71	Joback Method
dvisc	0.0011778	Pa×s	312.96	Joback Method
dvisc	0.0007450	Pa×s	347.21	Joback Method
dvisc	0.0005117	Pa×s	381.46	Joback Method
dvisc	0.0003739	Pa×s	415.71	Joback Method
dvisc	0.0002866	Pa×s	449.96	Joback Method

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U132285&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point