CHLOROACETIC ACID, 2-METHYLPROPYL ESTER

Other names: Acetic acid, chloro-, 2-methylpropyl ester
Isobutyl chloroacetate
Inchi: InChI=1S/C6H11ClO2/c1-5(2)4-9-6(8)3-7/h5H,3-4H2,1-2H3
InchiKey: QSGCJQBBHYWZHS-UHFFFAOYSA-N
Formula: C6H11ClO2
SMILES: CC(C)COC(=O)CCl
Mol. weight [g/mol]: 150.61
CAS: 13361-35-8

Physical Properties

Property code	Value	Unit	Source
af	0.4650		Cheméo Relay (1.0)
chl	-3399.00	kJ/mol	NIST Webbook
hf	-522.77	kJ/mol	Cheméo Relay (1.0)
hfus	14.76	kJ/mol	Joback Method
hvap	40.00	kJ/mol	NIST Webbook
ie	10.31	eV	Cheméo Relay (1.0)
log10ws	-1.72		Cheméo Relay (1.0)
logp	1.424		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	956.00		NIST Webbook
rinpol	959.60		NIST Webbook
rinpol	959.60		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	956.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1392.00		NIST Webbook
tb	442.68	K	Cheméo Relay (1.0)
tc	623.34	K	Cheméo Relay (1.0)
tf	237.41	K	Cheméo Relay (1.0)
vc	0.419	m3/kmol	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	278.93	J/mol×K	638.50	Joback Method
cpg	270.88	J/mol×K	607.08	Joback Method
cpg	262.46	J/mol×K	575.65	Joback Method
cpg	253.66	J/mol×K	544.23	Joback Method
cpg	244.50	J/mol×K	512.81	Joback Method
cpg	234.96	J/mol×K	481.38	Joback Method
dvisc	0.0007450	Pa×s	347.21	Joback Method
dvisc	0.0002866	Pa×s	449.96	Joback Method
dvisc	0.0003739	Pa×s	415.71	Joback Method
dvisc	0.0005117	Pa×s	381.46	Joback Method
dvisc	0.0043249	Pa×s	244.46	Joback Method
dvisc	0.0011778	Pa×s	312.96	Joback Method
dvisc	0.0020836	Pa×s	278.71	Joback Method
hvapt	43.90	kJ/mol	308.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.12750e+01
Coeff. B	-2.75686e+03
Coeff. C	-6.61400e+01
Temperature range (K), min.	293.00
Temperature range (K), max.	528.42

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13361358&Units=SI

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume