METHYL CIS-3-CHLOROPROPENOATE

Other names: Methyl (Z)-3-chloropropenoate
cis-3-chloropropenoic acid, methyl ester
Inchi: InChI=1S/C4H5ClO2/c1-7-4(6)2-3-5/h2-3H,1H3
InchiKey: ZLDNFLVIPPOXQL-IHWYPQMZSA-N
Formula: C4H5ClO2
SMILES: COC(=O)/C=C\Cl
Mol. weight [g/mol]: 120.53

Physical Properties

Property code	Value	Unit	Source
af	0.3671		Cheméo Relay (1.0)
hf	-324.05	kJ/mol	Cheméo Relay (1.0)
hfus	13.30	kJ/mol	Joback Method
hvap	46.65	kJ/mol	Cheméo Relay (1.0)
ie	10.15	eV	Cheméo Relay (1.0)
log10ws	-1.55		Cheméo Relay (1.0)
logp	0.912		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
rinpol	802.00		NIST Webbook
rinpol	802.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1374.00		NIST Webbook
ripol	1382.00		NIST Webbook
tb	415.50	K	Cheméo Relay (1.0)
tc	603.38	K	Cheméo Relay (1.0)
tf	203.57	K	Cheméo Relay (1.0)
vc	0.281	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.25	J/mol×K	408.80	Joback Method
cpg	141.57	J/mol×K	441.69	Joback Method

cpg	147.60	J/mol×K	474.57	Joback Method
cpg	153.36	J/mol×K	507.46	Joback Method
cpg	158.85	J/mol×K	540.35	Joback Method
cpg	164.07	J/mol×K	573.24	Joback Method
cpg	169.05	J/mol×K	606.12	Joback Method
dvisc	0.0025428	Pa×s	231.84	Joback Method
dvisc	0.0014158	Pa×s	261.33	Joback Method
dvisc	0.0008877	Pa×s	290.83	Joback Method
dvisc	0.0006066	Pa×s	320.32	Joback Method
dvisc	0.0004420	Pa×s	349.81	Joback Method
dvisc	0.0003383	Pa×s	379.31	Joback Method
dvisc	0.0002691	Pa×s	408.80	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=U144787&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

af: Acentric Factor
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
vc:	Critical Volume