

trans Methyl 3-chloro-2-propenoate

Inchi:	InChI=1S/C4H5ClO2/c1-7-4(6)2-3-5/h2-3H,1H3/b3-2+
InchiKey:	ZLDNFLVIPPOXQL-NSCUHMNNSA-N
Formula:	C4H5ClO2
SMILES:	COC(=O)C=CCl
Mol. weight [g/mol]:	120.53
CAS:	5135-18-2

Physical Properties

Property code	Value	Unit	Source
gf	-182.83	kJ/mol	Joback Method
hf	-269.21	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	38.00	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.912		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	408.80	K	Joback Method
tc	606.12	K	Joback Method
tf	231.84	K	Joback Method
vc	0.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.25	J/molxK	408.80	Joback Method
cpg	141.57	J/molxK	441.69	Joback Method
cpg	147.60	J/molxK	474.57	Joback Method
cpg	153.36	J/molxK	507.46	Joback Method
cpg	158.85	J/molxK	540.35	Joback Method
cpg	164.07	J/molxK	573.24	Joback Method
cpg	169.05	J/molxK	606.12	Joback Method
dvisc	0.0025428	Paxs	231.84	Joback Method
dvisc	0.0014158	Paxs	261.33	Joback Method

dvisc	0.0008877	Paxs	290.83	Joback Method
dvisc	0.0006066	Paxs	320.32	Joback Method
dvisc	0.0004420	Paxs	349.81	Joback Method
dvisc	0.0003383	Paxs	379.31	Joback Method
dvisc	0.0002691	Paxs	408.80	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5135182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
vc:	Critical Volume

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