METHYL 3,3-DICHLOROPROPENOATE

Other names: 3,3-Dichloropropenoic acid, methyl ester
Inchi: InChI=1S/C4H4Cl2O2/c1-8-4(7)2-3(5)6/h2H,1H3
InchiKey: YPCKXQGCSGMTIR-UHFFFAOYSA-N
Formula: C4H4Cl2O2
SMILES: COC(=O)C=C(Cl)Cl
Mol. weight [g/mol]: 154.98

Physical Properties

Property code	Value	Unit	Source
af	0.3510		Cheméo Relay (1.0)
hf	-352.76	kJ/mol	Cheméo Relay (1.0)
hfus	16.19	kJ/mol	Joback Method
hvap	50.96	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-1.89		Cheméo Relay (1.0)
logp	1.478		Crippen Method
mcvol	94.840	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	916.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1382.00		NIST Webbook
tb	435.38	K	Cheméo Relay (1.0)
tc	616.73	K	Cheméo Relay (1.0)
tf	226.80	K	Cheméo Relay (1.0)
vc	0.328	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.02	J/mol×K	446.11	Joback Method

cpg	161.10	J/mol×K	480.88	Joback Method
cpg	166.85	J/mol×K	515.64	Joback Method
cpg	172.29	J/mol×K	550.41	Joback Method
cpg	177.42	J/mol×K	585.18	Joback Method
cpg	182.26	J/mol×K	619.95	Joback Method
cpg	186.82	J/mol×K	654.71	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2257467&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
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