

Methyl E-2,3-dichloropropenoate

Other names:	Methyl trans-2,3-dichloropropenoate trans-2,3-Dichloropropenoic acid, methyl ester
Inchi:	InChI=1S/C4H4Cl2O2/c1-8-4(7)3(6)2-5/h2H,1H3/b3-2+
InchiKey:	DHANPGDOODFCAZ-NSCUHMNNSA-N
Formula:	C4H4Cl2O2
SMILES:	COC(=O)C(Cl)=CCl
Mol. weight [g/mol]:	154.98
CAS:	3533-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-203.31	kJ/mol	Joback Method
hf	-294.74	kJ/mol	Joback Method
hfus	16.19	kJ/mol	Joback Method
hvap	42.46	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	1.478		Crippen Method
mvol	94.840	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
rinpol	919.00		NIST Webbook
rinpol	917.00		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1473.00		NIST Webbook
tb	446.11	K	Joback Method
tc	654.71	K	Joback Method
tf	247.80	K	Joback Method
vc	0.362	m ³ /kmol	Joback Method

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3533708&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
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

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