

Mucochloric acid

Other names:	Dichloromalealdehydic acid 2-Butenoic acid, 2,3-dichloro-4-oxo-, (Z)- «alpha», «beta»-Dichloro-«beta»-formylacrylic acid Acrylic acid, 2,3-dichloro-3-formyl- Kyselina mukochlorova 2,3-Dichloromaleic aldehyde acid Aldehydodichloromaleic acid 2-Butenoic acid, 2,3-dichlor-4-oxo-, (Z)- 3,4-Dichloro-2-hydroxycrotonolactone 3,4-Dichloro-2-hydroxycrotonolactonic acid 2,3-Dichloro-4-oxo-2-butenoic acid Malealdehydic acid, dichloro-4-oxo-, (Z)- 2-Butenoic acid, 2,3-dichloro-4-oxo-, (2Z)-
Inchi:	InChI=1S/C4H2Cl2O3/c5-2(1-7)3(6)4(8)9/h1H,(H,8,9)/b3-2+
InchiKey:	LUMLZKVIXLWTCI-NSCUHMNNSA-N
Formula:	C4H2Cl2O3
SMILES:	O=CC(Cl)=C(Cl)C(=O)O
Mol. weight [g/mol]:	168.96
CAS:	87-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-343.20	kJ/mol	Joback Method
hf	-410.12	kJ/mol	Joback Method
hfus	20.07	kJ/mol	Joback Method
hvap	63.53	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	0.959		Crippen Method
mcvol	96.410	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
tb	564.41	K	Joback Method
tc	769.16	K	Joback Method
tf	314.43	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.30	J/mol×K	564.41	Joback Method
cpg	178.47	J/mol×K	598.53	Joback Method
cpg	182.31	J/mol×K	632.66	Joback Method
cpg	185.85	J/mol×K	666.78	Joback Method
cpg	189.11	J/mol×K	700.91	Joback Method
cpg	192.12	J/mol×K	735.03	Joback Method
cpg	194.90	J/mol×K	769.16	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C87569&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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