

Propionic acid, 2,3,3-trichloro-2-chloromethyl, methyl ester

Inchi:	InChI=1S/C5H6Cl4O2/c1-4(6,3(10)11-2)5(7,8)9/h1-2H3
InchiKey:	SXFXYUOFMJTPS-UHFFFAOYSA-N
Formula:	C5H6Cl4O2
SMILES:	COC(=O)C(C)(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	239.91

Physical Properties

Property code	Value	Unit	Source
gf	-284.74	kJ/mol	Joback Method
hf	-471.79	kJ/mol	Joback Method
hfus	13.45	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.527		Crippen Method
mcvol	137.710	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	533.35	K	Joback Method
tc	763.67	K	Joback Method
tf	342.79	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.52	J/molxK	533.35	Joback Method
cpg	293.84	J/molxK	725.29	Joback Method
cpg	288.30	J/molxK	686.90	Joback Method
cpg	282.15	J/molxK	648.51	Joback Method
cpg	275.34	J/molxK	610.12	Joback Method
cpg	267.82	J/molxK	571.74	Joback Method
cpg	298.83	J/molxK	763.67	Joback Method
dvisc	0.0002759	Paxs	533.35	Joback Method
dvisc	0.0003632	Paxs	501.59	Joback Method
dvisc	0.0004962	Paxs	469.83	Joback Method

dvisc	0.0007093	Paxs	438.07	Joback Method
dvisc	0.0010723	Paxs	406.31	Joback Method
dvisc	0.0017387	Paxs	374.55	Joback Method
dvisc	0.0030833	Paxs	342.79	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=B6001955&Units=SI

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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