

Propanoic acid, 2,2,3,3-tetrachloro-, methyl ester

Inchi:	InChI=1S/C4H4Cl4O2/c1-10-3(9)4(7,8)2(5)6/h2H,1H3
InchiKey:	UQYYMXYSOOLLA-UHFFFAOYSA-N
Formula:	C4H4Cl4O2
SMILES:	COC(=O)C(Cl)(Cl)C(Cl)Cl
Mol. weight [g/mol]:	225.88
CAS:	20618-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-298.44	kJ/mol	Joback Method
hf	-447.68	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	49.51	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.137		Crippen Method
mcvol	123.620	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1156.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	513.26	K	Joback Method
tc	738.13	K	Joback Method
tf	314.10	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.59	J/molxK	513.26	Joback Method
cpg	243.95	J/molxK	700.65	Joback Method
cpg	239.23	J/molxK	663.17	Joback Method
cpg	234.07	J/molxK	625.69	Joback Method
cpg	228.42	J/molxK	588.22	Joback Method

cpg	222.27	J/mol×K	550.74	Joback Method
cpg	248.23	J/mol×K	738.13	Joback Method
dvisc	0.0003143	Paxs	513.26	Joback Method
dvisc	0.0004125	Paxs	480.07	Joback Method
dvisc	0.0005637	Paxs	446.87	Joback Method
dvisc	0.0008101	Paxs	413.68	Joback Method
dvisc	0.0012400	Paxs	380.49	Joback Method
dvisc	0.0020592	Paxs	347.29	Joback Method
dvisc	0.0038064	Paxs	314.10	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=C20618057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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