Trichloroacetic acid, propyl ester

Other names:	Acetic acid, trichloro-, propyl ester
	Propyl trichloroacetate
	n-Propyl trichloroacetate
Inchi:	InChI=1S/C5H7Cl3O2/c1-2-3-10-4(9)5(6,7)8/h2-3H2,1H3
InchiKey:	QWWBZHDIGCDTLY-UHFFFAOYSA-N
Formula:	C5H7Cl3O2
SMILES:	CCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	205.47
CAS:	13313-91-2

Physical Properties

Property code	Value	Unit	Source
chl	-2516.00	kJ/mol	NIST Webbook
chl	-2523.00 ± 8.40	kJ/mol	NIST Webbook
gf	-275.65	kJ/mol	Joback Method
hf	-460.20 ± 9.60	kJ/mol	NIST Webbook
hfl	-513.40 ± 8.40	kJ/mol	NIST Webbook
hfus	16.67	kJ/mol	Joback Method
hvap	53.10 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.34		Crippen Method
logp	2.310		Crippen Method
mcvol	125.470	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1026.00		NIST Webbook
rinpol	1051.20		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1064.00		NIST Webbook

ripol	1459.00		NIST Webbook
ripol	1471.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1512.00		NIST Webbook
tb	499.15	K	Joback Method
tc	710.20	K	Joback Method
tf	310.45	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.65	J/mol×K	499.15	Joback Method
cpg	243.00	J/mol×K	534.32	Joback Method
cpg	250.81	J/mol×K	569.50	Joback Method
cpg	258.10	J/mol×K	604.67	Joback Method
cpg	264.90	J/mol×K	639.85	Joback Method
cpg	271.22	J/mol×K	675.02	Joback Method
cpg	277.09	J/mol×K	710.20	Joback Method
dvisc	0.0032418	Pa×s	310.45	Joback Method
dvisc	0.0018441	Pa×s	341.90	Joback Method
dvisc	0.0011536	Pa×s	373.35	Joback Method
dvisc	0.0007762	Pa×s	404.80	Joback Method
dvisc	0.0005530	Pa×s	436.25	Joback Method
dvisc	0.0004123	Pa×s	467.70	Joback Method
dvisc	0.0003190	Pa×s	499.15	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=C13313912&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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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