

Trichloroacetic acid, 2,2-dimethylpropyl ester

Other names:	Trichloroacetic acid, neopentyl ester
Inchi:	InChI=1S/C7H11Cl3O2/c1-6(2,3)4-12-5(11)7(8,9)10/h4H2,1-3H3
InchiKey:	WCORDUWUJLFFJQ-UHFFFAOYSA-N
Formula:	C7H11Cl3O2
SMILES:	CC(C)(C)COC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	233.52
CAS:	57392-56-0

Physical Properties

Property code	Value	Unit	Source
gf	-255.97	kJ/mol	Joback Method
hf	-497.33	kJ/mol	Joback Method
hfus	14.44	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.946		Crippen Method
mcvol	153.650	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	541.68	K	Joback Method
tc	759.32	K	Joback Method
tf	335.41	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.35	J/molxK	541.68	Joback Method
cpg	333.60	J/molxK	577.95	Joback Method
cpg	344.01	J/molxK	614.23	Joback Method
cpg	353.63	J/molxK	650.50	Joback Method
cpg	362.50	J/molxK	686.77	Joback Method
cpg	370.68	J/molxK	723.04	Joback Method
cpg	378.22	J/molxK	759.32	Joback Method
dvisc	0.0033014	Paxs	335.41	Joback Method

dvisc	0.0017293	Paxs	369.79	Joback Method
dvisc	0.0010112	Paxs	404.17	Joback Method
dvisc	0.0006431	Paxs	438.55	Joback Method
dvisc	0.0004369	Paxs	472.92	Joback Method
dvisc	0.0003127	Paxs	507.30	Joback Method
dvisc	0.0002336	Paxs	541.68	Joback Method
hvapt	57.70	kJ/mol	425.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57392560&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
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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