

Phenol, pentachloro-, trichloroacetate

Other names:	Acetic acid, trichloro-, pentachlorophenyl ester Pentachlorophenyl trichloroacetate
Inchi:	InChI=1S/C8Cl8O2/c9-1-2(10)4(12)6(5(13)3(1)11)18-7(17)8(14,15)16
InchiKey:	WMUFBMFZOHGUPA-UHFFFAOYSA-N
Formula:	C8Cl8O2
SMILES:	O=C(Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	411.71
CAS:	2879-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-245.78	kJ/mol	Joback Method
hf	-408.74	kJ/mol	Joback Method
hfus	37.52	kJ/mol	Joback Method
hvap	81.93	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	6.229		Crippen Method
mvol	205.180	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
tb	806.52	K	Joback Method
tc	1070.07	K	Joback Method
tf	582.88	K	Joback Method
vc	0.780	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.67	J/mol×K	806.52	Joback Method
cpg	363.73	J/mol×K	850.45	Joback Method
cpg	367.21	J/mol×K	894.37	Joback Method
cpg	370.17	J/mol×K	938.30	Joback Method
cpg	372.62	J/mol×K	982.22	Joback Method
cpg	374.61	J/mol×K	1026.15	Joback Method
cpg	376.16	J/mol×K	1070.07	Joback Method

dvisc	0.0004047	Paxs	582.88	Joback Method
dvisc	0.0003026	Paxs	620.15	Joback Method
dvisc	0.0002338	Paxs	657.43	Joback Method
dvisc	0.0001858	Paxs	694.70	Joback Method
dvisc	0.0001511	Paxs	731.97	Joback Method
dvisc	0.0001253	Paxs	769.25	Joback Method
dvisc	0.0001058	Paxs	806.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2879609&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
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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