

Phenol, 2,3,5,6-tetrachloro-, acetate

Other names:	Acetic acid, 2,3,5,6-tetrachlorophenyl ester]Henol, 2,3,5,6-tetrachloro-, acetate
Inchi:	InChI=1S/C8H4Cl4O2/c1-3(13)14-8-6(11)4(9)2-5(10)7(8)12/h2H,1H3
InchiKey:	NHBOZDKIYJWIIT-UHFFFAOYSA-N
Formula:	C8H4Cl4O2
SMILES:	CC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	273.93
CAS:	61925-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-191.27	kJ/mol	Joback Method
hf	-325.56	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	65.02	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.226		Crippen Method
mcvol	156.220	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	1633.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1612.00		NIST Webbook
ripol	2225.00		NIST Webbook
tb	655.05	K	Joback Method
tc	895.37	K	Joback Method
tf	448.26	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.91	J/molxK	655.05	Joback Method
cpg	302.43	J/molxK	695.10	Joback Method
cpg	309.43	J/molxK	735.16	Joback Method

cpg	315.89	J/molxK	775.21	Joback Method
cpg	321.82	J/molxK	815.26	Joback Method
cpg	327.20	J/molxK	855.31	Joback Method
cpg	332.02	J/molxK	895.37	Joback Method
dvisc	0.0008237	Paxs	448.26	Joback Method
dvisc	0.0006042	Paxs	482.72	Joback Method
dvisc	0.0004619	Paxs	517.19	Joback Method
dvisc	0.0003652	Paxs	551.65	Joback Method
dvisc	0.0002968	Paxs	586.12	Joback Method
dvisc	0.0002468	Paxs	620.59	Joback Method
dvisc	0.0002093	Paxs	655.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61925904&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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