2,3,5-Trichlorophenol, acetate

Other names: Phenol, 2,3,5-trichloro, acetate
Inchi: InChI=1S/C8H5Cl3O2/c1-4(12)13-7-3-5(9)2-6(10)8(7)11/h2-3H,1H3
InchiKey: YHKQUZSHMROARS-UHFFFAOYSA-N
Formula: C8H5Cl3O2
SMILES: CC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 239.48

Physical Properties

Property code	Value	Unit	Source
gf	-169.71	kJ/mol	Joback Method
hf	-298.35	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.572		Crippen Method
mcvol	143.980	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1476.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1476.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2117.00		NIST Webbook
tb	612.64	K	Joback Method
tc	848.96	K	Joback Method
tf	405.82	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.62	J/mol×K	612.64	Joback Method
cpg	286.07	J/mol×K	652.03	Joback Method
cpg	293.97	J/mol×K	691.41	Joback Method

cpg	301.31	J/mol×K	730.80	Joback Method
cpg	308.11	J/mol×K	770.19	Joback Method
cpg	314.35	J/mol×K	809.58	Joback Method
cpg	320.04	J/mol×K	848.96	Joback Method
dvisc	0.0010302	Pa×s	405.82	Joback Method
dvisc	0.0007244	Pa×s	440.29	Joback Method
dvisc	0.0005361	Pa×s	474.76	Joback Method
dvisc	0.0004132	Pa×s	509.23	Joback Method
dvisc	0.0003292	Pa×s	543.70	Joback Method
dvisc	0.0002695	Pa×s	578.17	Joback Method
dvisc	0.0002256	Pa×s	612.64	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=U364907&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume