Phenol, 3,4-dichloro-, acetate

Other names: Acetic acid, 3,4-dichlorophenyl ester
Inchi: InChI=1S/C8H6Cl2O2/c1-5(11)12-6-2-3-7(9)8(10)4-6/h2-4H,1H3
InchiKey: OSKGYRIYNMZFSJ-UHFFFAOYSA-N
Formula: C8H6Cl2O2
SMILES: CC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 205.04
CAS: 17847-51-7

Physical Properties

Property code	Value	Unit	Source
gf	-148.15	kJ/mol	Joback Method
hf	-271.14	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.919		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1410.00		NIST Webbook
ripol	2072.00		NIST Webbook
tb	570.23	K	Joback Method
tc	801.88	K	Joback Method
tf	363.38	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.56	J/mol×K	570.23	Joback Method
cpg	267.98	J/mol×K	608.84	Joback Method

cpg	276.81	J/mol×K	647.45	Joback Method
cpg	285.07	J/mol×K	686.06	Joback Method
cpg	292.76	J/mol×K	724.66	Joback Method
cpg	299.89	J/mol×K	763.27	Joback Method
cpg	306.45	J/mol×K	801.88	Joback Method
dvisc	0.0013093	Pa×s	363.38	Joback Method
dvisc	0.0008718	Pa×s	397.86	Joback Method
dvisc	0.0006194	Pa×s	432.33	Joback Method
dvisc	0.0004628	Pa×s	466.81	Joback Method
dvisc	0.0003600	Pa×s	501.28	Joback Method
dvisc	0.0002892	Pa×s	535.75	Joback Method
dvisc	0.0002386	Pa×s	570.23	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17847517&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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