PHENOL, 2,3,6-TRICHLORO-, ACETATE

Other names: Acetic acid, 2,3,6-trichlorophenyl ester
Inchi: InChI=1S/C8H5Cl3O2/c1-4(12)13-8-6(10)3-2-5(9)7(8)11/h2-3H,1H3
InchiKey: NIXCFOKFBOFURO-UHFFFAOYSA-N
Formula: C8H5Cl3O2
SMILES: CC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 239.49

Physical Properties

Property code	Value	Unit	Source
hf	-353.87	kJ/mol	Cheméo Relay (1.0)
hfus	24.73	kJ/mol	Joback Method
hvap	74.45	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-3.83		Cheméo Relay (1.0)
logp	3.572		Crippen Method
mcvol	143.980	ml/mol	McGowan Method
rinpol	1463.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1463.00		NIST Webbook
ripol	2139.00		NIST Webbook
tb	526.32	K	Cheméo Relay (1.0)
tf	316.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.62	J/mol×K	612.64	Joback Method
cpg	320.04	J/mol×K	848.96	Joback Method
cpg	314.35	J/mol×K	809.58	Joback Method
cpg	308.11	J/mol×K	770.19	Joback Method
cpg	301.31	J/mol×K	730.80	Joback Method
cpg	293.97	J/mol×K	691.41	Joback Method
cpg	286.07	J/mol×K	652.03	Joback Method
dvisc	0.0004132	Pa×s	509.23	Joback Method

dvisc	0.0002256	Pa×s	612.64	Joback Method
dvisc	0.0002695	Pa×s	578.17	Joback Method
dvisc	0.0003292	Pa×s	543.70	Joback Method
dvisc	0.0010302	Pa×s	405.82	Joback Method
dvisc	0.0005361	Pa×s	474.76	Joback Method
dvisc	0.0007244	Pa×s	440.29	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61925879&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point