2,3,4,6-Tetrachlorophenyl acetate

Other names: Acetic acid, 2,3,4,6-tetrachlorophenyl ester
Inchi: InChI=1S/C8H4Cl4O2/c1-3(13)14-8-5(10)2-4(9)6(11)7(8)12/h2H,1H3
InchiKey: RHZFLXLMXCNOHX-UHFFFAOYSA-N
Formula: C8H4Cl4O2
SMILES: CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 273.93
CAS: 5435-60-9

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	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1617.00		NIST Webbook
ripol	2236.00		NIST Webbook
ripol	2236.00		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/mol×K	655.05	Joback Method

cpg	302.43	J/mol×K	695.10	Joback Method
cpg	309.43	J/mol×K	735.16	Joback Method
cpg	315.89	J/mol×K	775.21	Joback Method
cpg	321.82	J/mol×K	815.26	Joback Method
cpg	327.20	J/mol×K	855.31	Joback Method
cpg	332.02	J/mol×K	895.37	Joback Method
dvisc	0.0008237	Pa×s	448.26	Joback Method
dvisc	0.0006042	Pa×s	482.72	Joback Method
dvisc	0.0004619	Pa×s	517.19	Joback Method
dvisc	0.0003652	Pa×s	551.65	Joback Method
dvisc	0.0002968	Pa×s	586.12	Joback Method
dvisc	0.0002468	Pa×s	620.59	Joback Method
dvisc	0.0002093	Pa×s	655.05	Joback Method

Sources

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=C5435609&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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