

Acetoxyacetic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C10H6Cl4O4/c1-4(15)17-3-7(16)18-10-6(12)2-5(11)8(13)9(10)14/h2H,3H2,1H3
InchiKey:	VMPFYBCJJFVALV-UHFFFAOYSA-N
Formula:	C10H6Cl4O4
SMILES:	CC(=O)OCC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	331.96

Physical Properties

Property code	Value	Unit	Source
gf	-408.35	kJ/mol	Joback Method
hf	-611.64	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	78.63	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.769		Crippen Method
mcvol	191.840	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinsol	2034.00		NIST Webbook
tb	777.10	K	Joback Method
tc	1010.28	K	Joback Method
tf	542.96	K	Joback Method
vc	0.732	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.83	J/molxK	777.10	Joback Method
cpg	425.74	J/molxK	815.96	Joback Method
cpg	432.89	J/molxK	854.83	Joback Method
cpg	439.28	J/molxK	893.69	Joback Method
cpg	444.88	J/molxK	932.55	Joback Method
cpg	449.67	J/molxK	971.41	Joback Method
cpg	453.64	J/molxK	1010.28	Joback Method
dvisc	0.0005124	Paxs	542.96	Joback Method
dvisc	0.0003762	Paxs	581.98	Joback Method

dvisc	0.0002871	Paxs	621.01	Joback Method
dvisc	0.0002263	Paxs	660.03	Joback Method
dvisc	0.0001831	Paxs	699.05	Joback Method
dvisc	0.0001515	Paxs	738.08	Joback Method
dvisc	0.0001278	Paxs	777.10	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=U355702&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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