

Acetoxyacetic acid, 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C10H7Cl3O4/c1-5(14)16-4-10(15)17-9-3-7(12)6(11)2-8(9)13/h2-3H,4H2,1H3
InchiKey:	SWGZAKBXZHMWLP-UHFFFAOYSA-N
Formula:	C10H7Cl3O4
SMILES:	CC(=O)OCC(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	297.52

Physical Properties

Property code	Value	Unit	Source
gf	-386.79	kJ/mol	Joback Method
hf	-584.43	kJ/mol	Joback Method
hfus	32.70	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.115		Crippen Method
mcvol	179.600	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinqol	1901.00		NIST Webbook
tb	734.69	K	Joback Method
tc	964.57	K	Joback Method
tf	500.52	K	Joback Method
vc	0.682	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.04	J/molxK	734.69	Joback Method
cpg	409.98	J/molxK	773.00	Joback Method
cpg	418.19	J/molxK	811.32	Joback Method
cpg	425.65	J/molxK	849.63	Joback Method
cpg	432.35	J/molxK	887.94	Joback Method
cpg	438.27	J/molxK	926.26	Joback Method
cpg	443.41	J/molxK	964.57	Joback Method
dvisc	0.0006523	Paxs	500.52	Joback Method
dvisc	0.0004623	Paxs	539.55	Joback Method

dvisc	0.0003432	Paxs	578.58	Joback Method
dvisc	0.0002646	Paxs	617.61	Joback Method
dvisc	0.0002104	Paxs	656.63	Joback Method
dvisc	0.0001716	Paxs	695.66	Joback Method
dvisc	0.0001431	Paxs	734.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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