

Acetoxyacetic acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C10H9ClO4/c1-7(12)14-6-10(13)15-9-4-2-8(11)3-5-9/h2-5H,6H2,1H3
InchiKey:	XDEZQKYHBPNTOE-UHFFFAOYSA-N
Formula:	C10H9ClO4
SMILES:	CC(=O)OCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	228.63

Physical Properties

Property code	Value	Unit	Source
gf	-343.67	kJ/mol	Joback Method
hf	-530.01	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	63.49	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.808		Crippen Method
mcvol	155.120	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1553.00		NIST Webbook
tb	649.87	K	Joback Method
tc	872.33	K	Joback Method
tf	415.64	K	Joback Method
vc	0.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.16	J/molxK	649.87	Joback Method
cpg	373.21	J/molxK	686.95	Joback Method
cpg	383.52	J/molxK	724.02	Joback Method
cpg	393.11	J/molxK	761.10	Joback Method
cpg	401.95	J/molxK	798.18	Joback Method
cpg	410.05	J/molxK	835.25	Joback Method
cpg	417.40	J/molxK	872.33	Joback Method
dvisc	0.0011091	Paxs	415.64	Joback Method
dvisc	0.0007125	Paxs	454.68	Joback Method

dvisc	0.0004909	Paxs	493.72	Joback Method
dvisc	0.0003572	Paxs	532.75	Joback Method
dvisc	0.0002715	Paxs	571.79	Joback Method
dvisc	0.0002137	Paxs	610.83	Joback Method
dvisc	0.0001731	Paxs	649.87	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=U307540&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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