

Acetic acid, 2-chlorophenyl ester

Other names:	o-Acetoxychlorobenzene o-Chlorophenyl acetate Acetic acid, o-chlorophenyl ester Phenol, o-chloro-, acetate o-Chlorofenylester kyseliny octove 2-Chlorophenyl acetate o-Chlorofenylester kyseliny octove (czech)
Inchi:	InChI=1S/C8H7ClO2/c1-6(10)11-8-5-3-2-4-7(8)9/h2-5H,1H3
InchiKey:	CJPVPOYTTALCNX-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	CC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	170.59
CAS:	4525-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-126.59	kJ/mol	Joback Method
hf	-243.93	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
ie	8.67 ± 0.03	eV	NIST Webbook
log10ws	-2.47		Crippen Method
logp	2.265		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1173.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1199.00		NIST Webbook
ripol	1829.00		NIST Webbook
tb	527.82	K	Joback Method
tc	753.98	K	Joback Method
tf	320.94	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.52	J/molxK	527.82	Joback Method
cpg	283.61	J/molxK	716.28	Joback Method
cpg	275.58	J/molxK	678.59	Joback Method
cpg	266.97	J/molxK	640.90	Joback Method
cpg	257.76	J/molxK	603.21	Joback Method
cpg	247.94	J/molxK	565.51	Joback Method
cpg	291.07	J/molxK	753.98	Joback Method
dvisc	0.0002456	Paxs	527.82	Joback Method
dvisc	0.0003030	Paxs	493.34	Joback Method
dvisc	0.0003857	Paxs	458.86	Joback Method
dvisc	0.0005107	Paxs	424.38	Joback Method
dvisc	0.0007106	Paxs	389.90	Joback Method
dvisc	0.0010543	Paxs	355.42	Joback Method
dvisc	0.0017026	Paxs	320.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4525751&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
ie:	Ionization energy
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

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