

Acetic acid, chloro-, phenyl ester

Other names:	Phenyl chloroacetate Chloroacetic acid, phenyl ester
Inchi:	InChI=1S/C8H7ClO2/c9-6-8(10)11-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	AGUWUIVKDXDKBT-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	O=C(CCl)Oc1ccccc1
Mol. weight [g/mol]:	170.59
CAS:	620-73-5

Physical Properties

Property code	Value	Unit	Source
gf	-116.96	kJ/mol	Joback Method
hf	-232.46	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.831		Crippen Method
mvol	119.500	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	522.84	K	Joback Method
tc	747.81	K	Joback Method
tf	308.42	K	Joback Method
vc	0.449	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.13	J/mol×K	522.84	Joback Method
cpg	248.91	J/mol×K	560.34	Joback Method
cpg	259.02	J/mol×K	597.83	Joback Method
cpg	268.46	J/mol×K	635.33	Joback Method
cpg	277.26	J/mol×K	672.82	Joback Method
cpg	285.43	J/mol×K	710.32	Joback Method
cpg	292.99	J/mol×K	747.81	Joback Method

dvisc	0.0022365	Paxs	308.42	Joback Method
dvisc	0.0012890	Paxs	344.16	Joback Method
dvisc	0.0008240	Paxs	379.89	Joback Method
dvisc	0.0005689	Paxs	415.63	Joback Method
dvisc	0.0004165	Paxs	451.37	Joback Method
dvisc	0.0003192	Paxs	487.10	Joback Method
dvisc	0.0002537	Paxs	522.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620735&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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