Chloroacetic acid, 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]: 170.60

Physical Properties

Property code	Value	Unit	Source
hf	-310.48	kJ/mol	Cheméo Relay (1.0)
hfus	17.50	kJ/mol	Joback Method
hvap	54.85	kJ/mol	Cheméo Relay (1.0)
ie	8.86	eV	Cheméo Relay (1.0)
log10ws	-2.25		Cheméo Relay (1.0)
logp	1.831		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
tb	502.90	K	Cheméo Relay (1.0)
tf	313.10	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.13	J/mol×K	522.84	Joback Method
cpg	292.99	J/mol×K	747.81	Joback Method
cpg	285.43	J/mol×K	710.32	Joback Method
cpg	277.26	J/mol×K	672.82	Joback Method
cpg	268.46	J/mol×K	635.33	Joback Method
cpg	259.02	J/mol×K	597.83	Joback Method
cpg	248.91	J/mol×K	560.34	Joback Method
dvisc	0.0005689	Pa×s	415.63	Joback Method
dvisc	0.0002537	Pa×s	522.84	Joback Method
dvisc	0.0003192	Pa×s	487.10	Joback Method
dvisc	0.0004165	Pa×s	451.37	Joback Method

dvisc	0.0022365	Pa×s	308.42	Joback Method
dvisc	0.0008240	Pa×s	379.89	Joback Method
dvisc	0.0012890	Pa×s	344.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620735&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point