

Chloroacetic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C9H9ClO3/c1-12-7-2-4-8(5-3-7)13-9(11)6-10/h2-5H,6H2,1H3
InchiKey:	CWZUOZZTNYZVSQ-UHFFFAOYSA-N
Formula:	C9H9ClO3
SMILES:	COc1ccc(OC(=O)CCl)cc1
Mol. weight [g/mol]:	200.62

Physical Properties

Property code	Value	Unit	Source
gf	-223.17	kJ/mol	Joback Method
hf	-396.79	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	54.52	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.839		Crippen Method
mvol	139.460	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1505.00		NIST Webbook
rinpol	1505.00		NIST Webbook
tb	573.12	K	Joback Method
tc	792.51	K	Joback Method
tf	354.44	K	Joback Method
vc	0.522	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.31	J/molxK	573.12	Joback Method
cpg	353.88	J/molxK	755.95	Joback Method
cpg	345.03	J/molxK	719.38	Joback Method
cpg	335.55	J/molxK	682.82	Joback Method
cpg	325.43	J/molxK	646.25	Joback Method
cpg	314.68	J/molxK	609.69	Joback Method
cpg	362.09	J/molxK	792.51	Joback Method
dvisc	0.0001851	Paxs	573.12	Joback Method

dvisc	0.0002291	Paxs	536.67	Joback Method
dvisc	0.0002926	Paxs	500.23	Joback Method
dvisc	0.0003883	Paxs	463.78	Joback Method
dvisc	0.0005409	Paxs	427.33	Joback Method
dvisc	0.0008013	Paxs	390.89	Joback Method
dvisc	0.0012872	Paxs	354.44	Joback Method

Sources

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=U307714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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