4-CHLOROPHENOXYACETIC ACID, METHYL,ESTER

Other names: Acetic acid, 4-chlorophenoxy, methyl ester
Inchi: InChI=1S/C9H9ClO3/c1-12-9(11)6-13-8-4-2-7(10)3-5-8/h2-5H,6H2,1H3
InchiKey: OSGZHKYFZSNKRI-UHFFFAOYSA-N
Formula: C9H9ClO3
SMILES: COC(=O)COc1ccc(Cl)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	-1.98		Crippen Method
logp	1.892		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	573.12	K	Joback Method
tc	792.51	K	Joback Method
tf	354.44	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.31	J/mol×K	573.12	Joback Method
cpg	314.68	J/mol×K	609.69	Joback Method
cpg	325.43	J/mol×K	646.25	Joback Method
cpg	335.55	J/mol×K	682.82	Joback Method
cpg	345.03	J/mol×K	719.38	Joback Method
cpg	353.88	J/mol×K	755.95	Joback Method
cpg	362.09	J/mol×K	792.51	Joback Method
dvisc	0.0012872	Pa×s	354.44	Joback Method
dvisc	0.0008013	Pa×s	390.89	Joback Method

dvisc	0.0005409	Pa×s	427.33	Joback Method
dvisc	0.0003883	Pa×s	463.78	Joback Method
dvisc	0.0002926	Pa×s	500.23	Joback Method
dvisc	0.0002291	Pa×s	536.67	Joback Method
dvisc	0.0001851	Pa×s	573.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U362945&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
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
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