Acetic acid, phenoxy-

Other names:	2-Phenoxyacetic acid
	Acetic acid, 2-phenoxy-
	Acide phenoxyacetique
	Glycolic acid, phenyl ether
	Glycollic acid phenyl ether
	NSC 9810
	POA
	Phenoxyacetic acid
	Phenoxyethanoic acid
	o-Phenylglycolic acid
Inchi:	InChI=1S/C8H8O3/c9-8(10)6-11-7-4-2-1-3-5-7/h1-5H,6H2,(H,9,10)
InchiKey:	LCPDWSOZIOUXRV-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	O=C(O)COc1ccccc1
Mol. weight [g/mol]:	152.15
CAS:	122-59-8

Physical Properties

Property code	Value	Unit	Source
gf	-241.85	kJ/mol	Joback Method
hf	-368.95	kJ/mol	Joback Method
hfus	17.39	kJ/mol	Joback Method
hvap	61.51	kJ/mol	Joback Method
log10ws	-1.10		Aqueous Solubility Prediction Method
logp	1.150		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	577.59	K	Joback Method
tc	781.86	K	Joback Method
tf	372.65	K	Aqueous Solubility Prediction Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.57	J/mol×K	577.59	Joback Method
cpg	268.05	J/mol×K	611.63	Joback Method
cpg	276.96	J/mol×K	645.68	Joback Method
cpg	285.33	J/mol×K	679.72	Joback Method
cpg	293.16	J/mol×K	713.77	Joback Method
cpg	300.47	J/mol×K	747.81	Joback Method
cpg	307.28	J/mol×K	781.86	Joback Method
dvisc	0.0046046	Pa×s	339.32	Joback Method
dvisc	0.0017223	Pa×s	379.03	Joback Method
dvisc	0.0007763	Pa×s	418.74	Joback Method
dvisc	0.0004017	Pa×s	458.46	Joback Method
dvisc	0.0002309	Pa×s	498.17	Joback Method
dvisc	0.0001440	Pa×s	537.88	Joback Method
dvisc	0.0000958	Pa×s	577.59	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C122598&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubilities of cinnamic acid, phenoxyacetic acid and 4-methoxyphenylacetic acid in supercritical carbon dioxide: https://www.doi.org/10.1016/j.fluid.2008.09.009

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