2,3,4,5,6-Pentafluorophenoxy acetic acid

Other names:	Pentafluorophenoxyacetic acid
	Acetic acid, (pentafluorophenoxy)-
Inchi:	InChI=1S/C8H3F5O3/c9-3-4(10)6(12)8(7(13)5(3)11)16-1-2(14)15/h1H2,(H,14,15)
InchiKey:	SMXPFEBIAASLOR-UHFFFAOYSA-N
Formula:	C8H3F5O3
SMILES:	O=C(O)COc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	242.10
CAS:	14892-14-9

Physical Properties

Property code	Value	Unit	Source
gf	-1264.05	kJ/mol	Joback Method
hf	-1406.85	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	1.845		Crippen Method
mcvol	121.980	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	598.84	K	Joback Method
tc	768.33	K	Joback Method
tf	404.87	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.76	J/mol×K	598.84	Joback Method
cpg	300.32	J/mol×K	627.09	Joback Method
cpg	306.62	J/mol×K	655.34	Joback Method
cpg	312.65	J/mol×K	683.59	Joback Method
cpg	318.40	J/mol×K	711.83	Joback Method
cpg	323.87	J/mol×K	740.08	Joback Method
cpg	329.04	J/mol×K	768.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14892149&Units=SI

Legend

cpg:	Ideal gas heat capacity
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