p-Fluorophenoxyacetic acid

Other names:	4-Fluorophenoxyacetic acid
	Acetic acid, (4-fluorophenoxy)-
Inchi:	InChI=1S/C8H7FO3/c9-6-1-3-7(4-2-6)12-5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	ZBIULCVFFJJYTN-UHFFFAOYSA-N
Formula:	C8H7FO3
SMILES:	O=C(O)COc1ccc(F)cc1
Mol. weight [g/mol]:	170.14
CAS:	405-79-8

Physical Properties

Property code	Value	Unit	Source
gf	-446.29	kJ/mol	Joback Method
hf	-576.53	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.289		Crippen Method
mcvol	114.900	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	581.84	K	Joback Method
tc	777.80	K	Joback Method
tf	352.43	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.76	J/mol×K	581.84	Joback Method
cpg	274.54	J/mol×K	614.50	Joback Method
cpg	282.83	J/mol×K	647.16	Joback Method
cpg	290.65	J/mol×K	679.82	Joback Method
cpg	298.01	J/mol×K	712.48	Joback Method
cpg	304.90	J/mol×K	745.14	Joback Method
cpg	311.34	J/mol×K	777.80	Joback Method

Sources

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=C405798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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