2,3,4,5,6-Pentafluorophenylacetic acid

Other names:	Pentafluorophenylacetic acid
	Benzeneacetic acid, 2,3,4,5,6-pentafluoro-
Inchi:	InChI=1S/C8H3F5O2/c9-4-2(1-3(14)15)5(10)7(12)8(13)6(4)11/h1H2,(H,14,15)
InchiKey:	LGCODSNZJOVMHV-UHFFFAOYSA-N
Formula:	C8H3F5O2
SMILES:	O=C(O)Cc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	226.10
CAS:	653-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-1159.05	kJ/mol	Joback Method
hf	-1274.63	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	58.33	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.009		Crippen Method
mcvol	116.110	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	576.42	K	Joback Method
tc	746.06	K	Joback Method
tf	382.64	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.90	J/mol×K	576.42	Joback Method
cpg	279.38	J/mol×K	604.69	Joback Method
cpg	285.58	J/mol×K	632.97	Joback Method
cpg	291.51	J/mol×K	661.24	Joback Method
cpg	297.15	J/mol×K	689.51	Joback Method
cpg	302.52	J/mol×K	717.78	Joback Method
cpg	307.61	J/mol×K	746.06	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=C653214&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
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