«alpha»-Fluorophenylacetic acid

Other names: Benzeneacetic acid, «alpha»-fluoro-
fluorophenylacetic acid
Inchi: InChI=1S/C8H7FO2/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7H,(H,10,11)
InchiKey: ATPPNMLQNZHDOG-UHFFFAOYSA-N
Formula: C8H7FO2
SMILES: O=C(O)C(F)c1ccccc1
Mol. weight [g/mol]: 154.14
CAS: 1578-63-8

Physical Properties

Property code	Value	Unit	Source
gf	-334.10	kJ/mol	Joback Method
hf	-438.12	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	57.90	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.782		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	554.00	K	Joback Method
tc	754.67	K	Joback Method
tf	302.68	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.50	J/mol×K	554.00	Joback Method
cpg	254.88	J/mol×K	587.45	Joback Method
cpg	263.65	J/mol×K	620.89	Joback Method
cpg	271.85	J/mol×K	654.34	Joback Method
cpg	279.49	J/mol×K	687.78	Joback Method
cpg	286.60	J/mol×K	721.23	Joback Method
cpg	293.21	J/mol×K	754.67	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=C1578638&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