3-(4-Fluorophenyl)propionic acid

Inchi: InChI=1S/C9H9FO2/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-2,4-5H,3,6H2,(H,11,12)
InchiKey: ZMKXWDPUXLPHCA-UHFFFAOYSA-N
Formula: C9H9FO2
SMILES: O=C(O)CCc1ccc(F)cc1
Mol. weight [g/mol]: 168.16
CAS: 459-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-332.87	kJ/mol	Joback Method
hf	-464.95	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	61.17	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.843		Crippen Method
mcvol	123.120	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	582.30	K	Joback Method
tc	777.28	K	Joback Method
tf	341.47	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.69	J/mol×K	582.30	Joback Method
cpg	298.45	J/mol×K	614.80	Joback Method
cpg	307.65	J/mol×K	647.29	Joback Method
cpg	316.30	J/mol×K	679.79	Joback Method
cpg	324.43	J/mol×K	712.28	Joback Method
cpg	332.05	J/mol×K	744.78	Joback Method
cpg	339.19	J/mol×K	777.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C459314&Units=SI
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

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