3-(3-Fluoro-para-anisoyl)-propionic acid

Other names:	3-(3-Fluoro-4-methoxybenzoyl)propionic acid
	Benzenebutanoic acid, 3-fluoro-4-methoxy-«gamma»-oxo-
	3-(3'-Fluoro-p-anisoyl)propionic acid
Inchi:	InChI=1S/C11H11FO4/c1-16-10-4-2-7(6-8(10)12)9(13)3-5-11(14)15/h2,4,6H,3,5H2,1H3,(
InchiKey:	SNRFVYKMDZSFED-UHFFFAOYSA-N
Formula:	C11H11FO4
SMILES:	COc1ccc(C(=O)CCC(=O)O)cc1F
Mol. weight [g/mol]:	226.20
CAS:	347-63-7

Physical Properties

Property code	Value	Unit	Source
gf	-559.58	kJ/mol	Joback Method
hf	-762.50	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	75.44	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.882		Crippen Method
mcvol	158.740	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	709.33	K	Joback Method
tc	906.44	K	Joback Method
tf	448.69	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.01	J/mol×K	709.33	Joback Method
cpg	427.87	J/mol×K	742.18	Joback Method
cpg	437.12	J/mol×K	775.03	Joback Method
cpg	445.75	J/mol×K	807.89	Joback Method
cpg	453.79	J/mol×K	840.74	Joback Method
cpg	461.24	J/mol×K	873.59	Joback Method

cpg	468.10	J/mol×K	906.44	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=C347637&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