3-Fluoro-4-methoxyphenylacetic acid

Other names: Benzeneacetic acid, 3-fluoro-4-methoxy-
Inchi: InChI=1S/C9H9FO3/c1-13-8-3-2-6(4-7(8)10)5-9(11)12/h2-4H,5H2,1H3,(H,11,12)
InchiKey: VURNBRZIFABCRU-UHFFFAOYSA-N
Formula: C9H9FO3
SMILES: COc1ccc(CC(=O)O)cc1F
Mol. weight [g/mol]: 184.16
CAS: 452-14-2

Physical Properties

Property code	Value	Unit	Source
gf	-447.50	kJ/mol	Joback Method
hf	-608.64	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.461		Crippen Method
mcvol	128.990	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	609.70	K	Joback Method
tc	804.10	K	Joback Method
tf	376.22	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.08	J/mol×K	609.70	Joback Method
cpg	319.55	J/mol×K	642.10	Joback Method
cpg	328.52	J/mol×K	674.50	Joback Method
cpg	337.00	J/mol×K	706.90	Joback Method
cpg	345.00	J/mol×K	739.30	Joback Method
cpg	352.52	J/mol×K	771.70	Joback Method
cpg	359.57	J/mol×K	804.10	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=C452142&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