3-Fluorobenzoic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C14H11FO3/c1-17-12-5-7-13(8-6-12)18-14(16)10-3-2-4-11(15)9-10/h2-9H,1H3
InchiKey: ZBFPQPBBCXQLRA-UHFFFAOYSA-N
Formula: C14H11FO3
SMILES: COc1ccc(OC(=O)c2cccc(F)c2)cc1
Mol. weight [g/mol]: 246.23

Physical Properties

Property code	Value	Unit	Source
gf	-261.17	kJ/mol	Joback Method
hf	-455.30	kJ/mol	Joback Method
hfus	26.38	kJ/mol	Joback Method
hvap	63.38	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.054		Crippen Method
mcvol	175.680	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1861.00		NIST Webbook
rinpol	1861.00		NIST Webbook
tb	681.02	K	Joback Method
tc	910.83	K	Joback Method
tf	420.40	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.99	J/mol×K	681.02	Joback Method
cpg	460.77	J/mol×K	719.32	Joback Method
cpg	473.53	J/mol×K	757.62	Joback Method
cpg	485.28	J/mol×K	795.93	Joback Method
cpg	496.05	J/mol×K	834.23	Joback Method
cpg	505.83	J/mol×K	872.53	Joback Method
cpg	514.66	J/mol×K	910.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307727&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume