3-Fluorobenzoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C13H17FO3/c1-10(6-7-16-2)9-17-13(15)11-4-3-5-12(14)8-11/h3-5,8,10H,6-7,9

InchiKey: BZIRZKZQTYWOSX-UHFFFAOYSA-N

Formula: C13H17FO3

SMILES: COCCC(C)COC(=O)c1cccc(F)c1

Mol. weight [g/mol]: 240.27

Physical Properties

Property code	Value	Unit	Source
gf	-374.81	kJ/mol	Joback Method
hf	-665.00	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.655		Crippen Method
mcvol	185.350	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	626.04	K	Joback Method
tc	823.10	K	Joback Method
tf	355.19	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.93	J/mol×K	626.04	Joback Method
cpg	492.83	J/mol×K	658.88	Joback Method
cpg	506.94	J/mol×K	691.73	Joback Method
cpg	520.26	J/mol×K	724.57	Joback Method
cpg	532.81	J/mol×K	757.41	Joback Method
cpg	544.59	J/mol×K	790.26	Joback Method
cpg	555.60	J/mol×K	823.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355665&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

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