4-Fluorobenzoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C13H17FO2/c1-3-4-10(2)9-16-13(15)11-5-7-12(14)8-6-11/h5-8,10H,3-4,9H2,1-
InchiKey: CATGJDSHTUTNBU-UHFFFAOYSA-N
Formula: C13H17FO2
SMILES: CCCC(C)COC(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 224.27

Physical Properties

Property code	Value	Unit	Source
gf	-269.81	kJ/mol	Joback Method
hf	-532.78	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	55.42	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.419		Crippen Method
mcvol	179.480	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1534.00		NIST Webbook
tb	603.62	K	Joback Method
tc	802.32	K	Joback Method
tf	332.96	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.56	J/mol×K	603.62	Joback Method
cpg	466.76	J/mol×K	636.74	Joback Method
cpg	481.13	J/mol×K	669.85	Joback Method
cpg	494.70	J/mol×K	702.97	Joback Method
cpg	507.49	J/mol×K	736.09	Joback Method
cpg	519.51	J/mol×K	769.21	Joback Method
cpg	530.78	J/mol×K	802.32	Joback Method

Sources

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=U355675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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