3-Fluorobenzoic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C12H15FO2/c1-8(2)9(3)15-12(14)10-5-4-6-11(13)7-10/h4-9H,1-3H3
InchiKey: YPXFHPFYEYGJMI-UHFFFAOYSA-N
Formula: C12H15FO2
SMILES: CC(C)C(C)OC(=O)c1cccc(F)c1
Mol. weight [g/mol]: 210.24

Physical Properties

Property code	Value	Unit	Source
gf	-280.67	kJ/mol	Joback Method
hf	-517.42	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	52.81	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.027		Crippen Method
mcvol	165.390	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1389.00		NIST Webbook
tb	580.30	K	Joback Method
tc	785.94	K	Joback Method
tf	306.69	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.71	J/mol×K	580.30	Joback Method
cpg	417.62	J/mol×K	614.57	Joback Method
cpg	431.70	J/mol×K	648.85	Joback Method
cpg	444.97	J/mol×K	683.12	Joback Method
cpg	457.46	J/mol×K	717.39	Joback Method
cpg	469.17	J/mol×K	751.67	Joback Method
cpg	480.12	J/mol×K	785.94	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=U355660&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

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