3-fluorobenzoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C12H13FO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-6,8H,7H2,1-2H3
InchiKey: FFMWJRQUVVMAAC-UHFFFAOYSA-N
Formula: C12H13FO2
SMILES: CC(C)=CCOC(=O)c1cccc(F)c1
Mol. weight [g/mol]: 208.23

Physical Properties

Property code	Value	Unit	Source
hfus	25.25	kJ/mol	Joback Method
ie	8.94	eV	Cheméo Relay (1.0)
logp	2.949		Crippen Method
mcvol	161.090	ml/mol	McGowan Method
rinpol	1475.30		NIST Webbook
rinpol	1475.30		NIST Webbook
tb	525.20	K	Cheméo Relay (1.0)
tf	270.44	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.89	J/mol×K	585.22	Joback Method
cpg	395.78	J/mol×K	620.13	Joback Method
cpg	408.85	J/mol×K	655.04	Joback Method
cpg	421.14	J/mol×K	689.94	Joback Method
cpg	432.66	J/mol×K	724.85	Joback Method
cpg	443.46	J/mol×K	759.76	Joback Method
cpg	453.56	J/mol×K	794.67	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C154559383&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point