4-Fluorobenzoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C12H13FO2/c1-9(2)7-8-15-12(14)10-3-5-11(13)6-4-10/h3-7H,8H2,1-2H3
InchiKey: AAPZRXZXZNILPP-UHFFFAOYSA-N
Formula: C12H13FO2
SMILES: CC(C)=CCOC(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 208.23

Physical Properties

Property code	Value	Unit	Source
gf	-204.12	kJ/mol	Joback Method
hf	-399.43	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.949		Crippen Method
mcvol	161.090	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
tb	585.22	K	Joback Method
tc	794.67	K	Joback Method
tf	317.65	K	Joback Method
vc	0.623	m3/kmol	Joback Method

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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299151&Units=SI

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