3-Fluorobenzoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C15H19FO2/c1-3-4-5-6-8-12(2)18-15(17)13-9-7-10-14(16)11-13/h6-12H,3-5H2
InchiKey: QXBXJYCAVCJNTO-SOFGYWHQSA-N
Formula: C15H19FO2
SMILES: CCCCC=CC(C)OC(=O)c1cccc(F)c1
Mol. weight [g/mol]: 250.31

Physical Properties

Property code	Value	Unit	Source
gf	-172.75	kJ/mol	Joback Method
hf	-456.84	kJ/mol	Joback Method
hfus	30.80	kJ/mol	Joback Method
hvap	59.83	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.117		Crippen Method
mcvol	203.360	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1665.60		NIST Webbook
tb	653.54	K	Joback Method
tc	854.55	K	Joback Method
tf	350.42	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.01	J/mol×K	653.54	Joback Method
cpg	548.73	J/mol×K	687.04	Joback Method
cpg	563.54	J/mol×K	720.54	Joback Method
cpg	577.46	J/mol×K	754.05	Joback Method
cpg	590.55	J/mol×K	787.55	Joback Method
cpg	602.83	J/mol×K	821.05	Joback Method
cpg	614.33	J/mol×K	854.55	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=U292604&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