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

Inchi: InChI=1S/C10H8ClFO2/c11-5-2-6-14-10(13)8-3-1-4-9(12)7-8/h1-5,7H,6H2/b5-2+

InchiKey: QFKWMFWKGJVMEP-GORDUTHDSA-N

Formula: C10H8ClFO2

SMILES: O=C(OC/C=C/Cl)c1cccc(F)c1

Mol. weight [g/mol]: 214.62

Physical Properties

Property code	Value	Unit	Source
hfus	25.57	kJ/mol	Joback Method
ie	9.46	eV	Cheméo Relay (1.0)
logp	2.735		Crippen Method
mcvol	145.150	ml/mol	McGowan Method
rinpol	1493.20		NIST Webbook
rinpol	1493.20		NIST Webbook
tb	524.67	K	Cheméo Relay (1.0)
tf	267.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.23	J/mol×K	577.01	Joback Method
cpg	325.45	J/mol×K	613.16	Joback Method
cpg	335.94	J/mol×K	649.31	Joback Method
cpg	345.73	J/mol×K	685.45	Joback Method
cpg	354.86	J/mol×K	721.60	Joback Method
cpg	363.34	J/mol×K	757.75	Joback Method
cpg	371.21	J/mol×K	793.90	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292610&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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