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

Inchi: InChI=1S/C10H8ClFO2/c11-6-1-7-14-10(13)8-2-4-9(12)5-3-8/h1-6H,7H2/b6-1+

InchiKey: SSUKEGHTTWEKSA-LZCJLJQNSA-N

Formula: C10H8ClFO2

SMILES: O=C(OCC=CCl)c1ccc(F)cc1

Mol. weight [g/mol]: 214.62

Physical Properties

Property code	Value	Unit	Source
gf	-224.34	kJ/mol	Joback Method
hf	-364.10	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	53.47	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.735		Crippen Method
mcvol	145.150	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
tb	577.01	K	Joback Method
tc	793.90	K	Joback Method
tf	338.99	K	Joback Method
vc	0.558	m3/kmol	Joback Method

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

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=U299160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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