

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:	QFKWMFWKGVMEP-GORDUTHDSA-N
Formula:	C10H8ClFO2
SMILES:	O=C(OCC=CCl)c1cccc(F)c1
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
rinpola	1493.20		NIST Webbook
rinpola	1493.20		NIST Webbook
tb	577.01	K	Joback Method
tc	793.90	K	Joback Method
tf	338.99	K	Joback Method
vc	0.558	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U292610&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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