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

Inchi: InChI=1S/C10H6ClF3O2/c11-4-1-5-16-10(15)6-2-3-7(12)9(14)8(6)13/h1-4H,5H2/b4-1+

InchiKey: GAXBRMYVJHBNHQ-DAFODLJHSA-N

Formula: C10H6ClF3O2

SMILES: O=C(OCC=CCl)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 250.60

Physical Properties

Property code	Value	Unit	Source
gf	-633.22	kJ/mol	Joback Method
hf	-779.26	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	53.16	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.013		Crippen Method
mcvol	148.690	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1485.40		NIST Webbook
rinpol	1485.40		NIST Webbook
tb	585.51	K	Joback Method
tc	784.59	K	Joback Method
tf	365.21	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.83	J/mol×K	585.51	Joback Method
cpg	338.49	J/mol×K	618.69	Joback Method
cpg	347.60	J/mol×K	651.87	Joback Method
cpg	356.18	J/mol×K	685.05	Joback Method
cpg	364.24	J/mol×K	718.23	Joback Method
cpg	371.80	J/mol×K	751.41	Joback Method
cpg	378.87	J/mol×K	784.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292561&Units=SI
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

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