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

Inchi: InChI=1S/C11H8ClF3O2/c12-5-2-6-17-10(16)8-3-1-4-9(7-8)11(13,14)15/h1-5,7H,6H2/b5-

InchiKey: PUYCTCTXIMUWRA-GORDUTHDSA-N

Formula: C11H8ClF3O2

SMILES: O=C(OCC=CCl)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 264.63

Physical Properties

Property code	Value	Unit	Source
gf	-602.70	kJ/mol	Joback Method
hf	-785.71	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	52.77	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.615		Crippen Method
mcvol	162.780	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
tb	595.20	K	Joback Method
tc	800.74	K	Joback Method
tf	353.86	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.52	J/mol×K	595.20	Joback Method
cpg	391.98	J/mol×K	629.46	Joback Method
cpg	402.62	J/mol×K	663.71	Joback Method
cpg	412.48	J/mol×K	697.97	Joback Method
cpg	421.60	J/mol×K	732.23	Joback Method
cpg	430.04	J/mol×K	766.48	Joback Method
cpg	437.85	J/mol×K	800.74	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299329&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
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