2,3,4-Trifluorobenzoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C15H17F3O2/c1-3-4-5-6-7-10(2)20-15(19)11-8-9-12(16)14(18)13(11)17/h6-10
InchiKey: ASZHXOARIHLQJH-VOTSOKGWSA-N
Formula: C15H17F3O2
SMILES: CCCCC=CC(C)OC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 286.29

Physical Properties

Property code	Value	Unit	Source
gf	-581.63	kJ/mol	Joback Method
hf	-872.00	kJ/mol	Joback Method
hfus	36.19	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.396		Crippen Method
mcvol	206.900	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	1650.90		NIST Webbook
tb	662.04	K	Joback Method
tc	849.55	K	Joback Method
tf	376.64	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.89	J/mol×K	662.04	Joback Method
cpg	562.02	J/mol×K	693.29	Joback Method
cpg	575.39	J/mol×K	724.54	Joback Method
cpg	588.03	J/mol×K	755.79	Joback Method
cpg	599.97	J/mol×K	787.04	Joback Method
cpg	611.23	J/mol×K	818.30	Joback Method
cpg	621.82	J/mol×K	849.55	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=U292555&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