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

Inchi: InChI=1S/C18H23F3O2/c1-2-3-4-5-6-7-8-9-10-13-23-18(22)14-11-12-15(19)17(21)16(14
InchiKey: PUQWGAJCMCBGJO-MDZDMXLPSA-N
Formula: C18H23F3O2
SMILES: CCCCCCCCC=CCOC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 328.37

Physical Properties

Property code	Value	Unit	Source
gf	-553.93	kJ/mol	Joback Method
hf	-928.64	kJ/mol	Joback Method
hfus	47.48	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.567		Crippen Method
mcvol	249.170	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	2045.80		NIST Webbook
rinpol	2045.80		NIST Webbook
tb	731.12	K	Joback Method
tc	913.92	K	Joback Method
tf	425.45	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.73	J/mol×K	731.12	Joback Method
cpg	724.99	J/mol×K	761.59	Joback Method
cpg	739.44	J/mol×K	792.05	Joback Method
cpg	753.10	J/mol×K	822.52	Joback Method
cpg	766.01	J/mol×K	852.99	Joback Method
cpg	778.18	J/mol×K	883.45	Joback Method
cpg	789.65	J/mol×K	913.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292559&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

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