2-Fluorobenzoic acid, undec-2-enyl ester

Inchi: InChI=1S/C18H25FO2/c1-2-3-4-5-6-7-8-9-12-15-21-18(20)16-13-10-11-14-17(16)19/h9-1
InchiKey: ZZIICTZUGZYCDV-FMIVXFBMSA-N
Formula: C18H25FO2
SMILES: CCCCCCCCC=CCOC(=O)c1ccccc1F
Mol. weight [g/mol]: 292.39

Physical Properties

Property code	Value	Unit	Source
gf	-145.05	kJ/mol	Joback Method
hf	-513.48	kJ/mol	Joback Method
hfus	42.10	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.289		Crippen Method
mcvol	245.630	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	722.62	K	Joback Method
tc	914.85	K	Joback Method
tf	399.23	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.16	J/mol×K	722.62	Joback Method
cpg	711.71	J/mol×K	754.66	Joback Method
cpg	727.34	J/mol×K	786.70	Joback Method
cpg	742.07	J/mol×K	818.74	Joback Method
cpg	755.94	J/mol×K	850.77	Joback Method
cpg	769.00	J/mol×K	882.81	Joback Method
cpg	781.28	J/mol×K	914.85	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=U299169&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