3-Fluorobenzoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C18H21FO2/c1-5-7-14(4)17(11-10-13(2)3)21-18(20)15-8-6-9-16(19)12-15/h6,8

InchiKey: IPPQQAMJZRJYKG-UHFFFAOYSA-N

Formula: C18H21FO2

SMILES: C=C(C)C#CC(OC(=O)c1cccc(F)c1)C(C)CCC

Mol. weight [g/mol]: 288.36

Physical Properties

Property code	Value	Unit	Source
gf	51.94	kJ/mol	Joback Method
hf	-253.32	kJ/mol	Joback Method
hfus	35.38	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.367		Crippen Method
mcvol	237.030	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	1829.30		NIST Webbook
tb	723.14	K	Joback Method
tc	938.59	K	Joback Method
tf	464.69	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.86	J/mol×K	723.14	Joback Method
cpg	665.65	J/mol×K	759.05	Joback Method
cpg	681.35	J/mol×K	794.96	Joback Method
cpg	696.01	J/mol×K	830.87	Joback Method
cpg	709.66	J/mol×K	866.77	Joback Method
cpg	722.34	J/mol×K	902.68	Joback Method
cpg	734.09	J/mol×K	938.59	Joback Method

Sources

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=U292607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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