3-Fluorobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C17H19FO2/c1-12(2)8-9-16(10-13(3)4)20-17(19)14-6-5-7-15(18)11-14/h5-7,11

InchiKey: BQKXOFJUHHXDMP-UHFFFAOYSA-N

Formula: C17H19FO2

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

Mol. weight [g/mol]: 274.33

Physical Properties

Property code	Value	Unit	Source
gf	43.52	kJ/mol	Joback Method
hf	-232.68	kJ/mol	Joback Method
hfus	32.79	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	3.977		Crippen Method
mcvol	222.940	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	1755.60		NIST Webbook
rinpol	1755.60		NIST Webbook
tb	700.26	K	Joback Method
tc	919.03	K	Joback Method
tf	453.42	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.55	J/mol×K	700.26	Joback Method
cpg	611.02	J/mol×K	736.72	Joback Method
cpg	626.43	J/mol×K	773.18	Joback Method
cpg	640.81	J/mol×K	809.64	Joback Method
cpg	654.19	J/mol×K	846.11	Joback Method
cpg	666.61	J/mol×K	882.57	Joback Method
cpg	678.11	J/mol×K	919.03	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=U292606&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

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