4-Fluorobenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C12H9FO2/c1-2-3-4-9-15-12(14)10-5-7-11(13)8-6-10/h1,3-8H,9H2
InchiKey: HSRWSEMQKACRHZ-UHFFFAOYSA-N
Formula: C12H9FO2
SMILES: C#CC=CCOC(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 204.20

Physical Properties

Property code	Value	Unit	Source
gf	27.50	kJ/mol	Joback Method
hf	-97.74	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	53.40	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.172		Crippen Method
mcvol	152.490	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1460.00		NIST Webbook
tb	575.46	K	Joback Method
tc	795.61	K	Joback Method
tf	378.58	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.59	J/mol×K	575.46	Joback Method
cpg	354.90	J/mol×K	612.15	Joback Method
cpg	366.39	J/mol×K	648.84	Joback Method
cpg	377.11	J/mol×K	685.54	Joback Method
cpg	387.09	J/mol×K	722.23	Joback Method
cpg	396.38	J/mol×K	758.92	Joback Method
cpg	405.02	J/mol×K	795.61	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=U299152&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