2-Fluorobenzoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C13H13FO2/c1-3-7-10(4-2)16-13(15)11-8-5-6-9-12(11)14/h5-6,8-10H,4H2,1-2
InchiKey: QOVPBZHWPOQSDK-UHFFFAOYSA-N
Formula: C13H13FO2
SMILES: CC#CC(CC)OC(=O)c1ccccc1F
Mol. weight [g/mol]: 220.24

Physical Properties

Property code	Value	Unit	Source
gf	-67.01	kJ/mol	Joback Method
hf	-260.48	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	57.57	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	2.784		Crippen Method
mcvol	170.880	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1537.00		NIST Webbook
tb	612.62	K	Joback Method
tc	834.59	K	Joback Method
tf	439.06	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.31	J/mol×K	612.62	Joback Method
cpg	425.81	J/mol×K	649.62	Joback Method
cpg	439.43	J/mol×K	686.61	Joback Method
cpg	452.20	J/mol×K	723.61	Joback Method
cpg	464.13	J/mol×K	760.60	Joback Method
cpg	475.25	J/mol×K	797.60	Joback Method
cpg	485.56	J/mol×K	834.59	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=U299164&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