2-Fluorobenzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C11H9FO2/c1-3-8(2)14-11(13)9-6-4-5-7-10(9)12/h1,4-8H,2H3
InchiKey: NETSIZKRMPIKBQ-UHFFFAOYSA-N
Formula: C11H9FO2
SMILES: C#CC(C)OC(=O)c1ccccc1F
Mol. weight [g/mol]: 192.19

Physical Properties

Property code	Value	Unit	Source
gf	-63.58	kJ/mol	Joback Method
hf	-199.60	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.004		Crippen Method
mcvol	142.700	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	547.98	K	Joback Method
tc	767.04	K	Joback Method
tf	357.39	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.15	J/mol×K	547.98	Joback Method
cpg	329.53	J/mol×K	584.49	Joback Method
cpg	341.15	J/mol×K	621.00	Joback Method
cpg	352.04	J/mol×K	657.51	Joback Method
cpg	362.22	J/mol×K	694.02	Joback Method
cpg	371.71	J/mol×K	730.53	Joback Method
cpg	380.53	J/mol×K	767.04	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=U299161&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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