2,6-difluorobenzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C11H8F2O2/c1-3-7(2)15-11(14)10-8(12)5-4-6-9(10)13/h1,4-7H,2H3
InchiKey: GDWZNZBLLTYAED-UHFFFAOYSA-N
Formula: C11H8F2O2
SMILES: C#CC(C)OC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 210.18

Physical Properties

Property code	Value	Unit	Source
hfus	25.91	kJ/mol	Joback Method
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-3.52		Cheméo Relay (1.0)
logp	2.143		Crippen Method
mcvol	144.470	ml/mol	McGowan Method
rinpol	1306.60		NIST Webbook
tf	292.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.87	J/mol×K	552.23	Joback Method
cpg	336.33	J/mol×K	587.12	Joback Method
cpg	347.13	J/mol×K	622.01	Joback Method
cpg	357.30	J/mol×K	656.90	Joback Method
cpg	366.85	J/mol×K	691.79	Joback Method
cpg	375.80	J/mol×K	726.68	Joback Method
cpg	384.16	J/mol×K	761.57	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292581&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point