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
gf	-268.02	kJ/mol	Joback Method
hf	-407.18	kJ/mol	Joback Method
hfus	25.91	kJ/mol	Joback Method
hvap	50.67	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.143		Crippen Method
mcvol	144.470	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1306.60		NIST Webbook
tb	552.23	K	Joback Method
tc	761.57	K	Joback Method
tf	370.50	K	Joback Method
vc	0.559	m3/kmol	Joback Method

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

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=U292581&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