2,3,4-trifluorobenzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C11H7F3O2/c1-3-6(2)16-11(15)7-4-5-8(12)10(14)9(7)13/h1,4-6H,2H3
InchiKey: FMXYCPDFVXHTHE-UHFFFAOYSA-N
Formula: C11H7F3O2
SMILES: C#CC(C)OC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 228.17

Physical Properties

Property code	Value	Unit	Source
hfus	28.60	kJ/mol	Joback Method
logp	2.282		Crippen Method
mcvol	146.240	ml/mol	McGowan Method
rinpol	1285.50		NIST Webbook
rinpol	1285.50		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.50	J/mol×K	556.48	Joback Method
cpg	343.12	J/mol×K	589.88	Joback Method
cpg	353.17	J/mol×K	623.28	Joback Method
cpg	362.68	J/mol×K	656.67	Joback Method
cpg	371.64	J/mol×K	690.07	Joback Method
cpg	380.08	J/mol×K	723.47	Joback Method
cpg	387.99	J/mol×K	756.87	Joback Method

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292551&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices