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

Inchi: InChI=1S/C13H11F3O2/c1-3-5-8(4-2)18-13(17)9-6-7-10(14)12(16)11(9)15/h6-8H,4H2,1-
InchiKey: GNXAAQHQJHHCOH-UHFFFAOYSA-N
Formula: C13H11F3O2
SMILES: CC#CC(CC)OC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 256.22

Physical Properties

Property code	Value	Unit	Source
hfus	33.93	kJ/mol	Joback Method
logp	3.063		Crippen Method
mcvol	174.420	ml/mol	McGowan Method
rinpol	1522.70		NIST Webbook
rinpol	1522.70		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.07	J/mol×K	621.12	Joback Method
cpg	438.79	J/mol×K	655.14	Joback Method
cpg	450.84	J/mol×K	689.16	Joback Method
cpg	462.22	J/mol×K	723.18	Joback Method
cpg	472.93	J/mol×K	757.21	Joback Method
cpg	482.97	J/mol×K	791.23	Joback Method
cpg	492.36	J/mol×K	825.25	Joback Method

Sources

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=U292554&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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