2,3,4-trifluorobenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H17F3O2/c1-4-5-6-11(9-10(2)3)21-16(20)12-7-8-13(17)15(19)14(12)18/h7

InchiKey: YMDLHXAODPRPKL-UHFFFAOYSA-N

Formula: C16H17F3O2

SMILES: CCC#CC(CC(C)C)OC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 298.30

Physical Properties

Property code	Value	Unit	Source
hfus	38.17	kJ/mol	Joback Method
logp	4.089		Crippen Method
mcvol	216.690	ml/mol	McGowan Method
rinpol	1698.40		NIST Webbook
rinpol	1698.40		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.49	J/mol×K	689.32	Joback Method
cpg	594.25	J/mol×K	722.63	Joback Method
cpg	608.16	J/mol×K	755.94	Joback Method
cpg	621.26	J/mol×K	789.25	Joback Method
cpg	633.54	J/mol×K	822.56	Joback Method
cpg	645.02	J/mol×K	855.87	Joback Method
cpg	655.72	J/mol×K	889.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292556&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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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