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Typical Product Specifications & Properties

2-Propenoic acid, 3-(4-methoxy-1-naphthalenyl)-, ethyl ester

CAS Number: : 15971-31-0

Specifications	Limits
Chemical Structure	 615610 615610_2-propenoic-acid-3-4-methoxy-1-naphthalenyl-ethyl-ester.png chemical structure
Chemical Structure	 chemicalStructure-2-propenoic-acid-3-4-methoxy-1-naphthalenyl-ethyl-ester
Molecular Formula	C16H16O3
Molecular weight	
Canonicalized Compound	1
Compound Complexity	324
Hydrogen Bond Acceptor Count	3
Hydrogen Bond Donor Count	
Rotatable Bond Count	5
Allowed IUPAC Name	ethyl (E)-3-(4-methoxy-1-naphthyl)prop-2-enoate
CAS-like Style IUPAC Name	(E)-3-(4-methoxy-1-naphthalenyl)-2-propenoic acid ethyl ester
Markup IUPAC Name	ethyl (<I>E</I>)-3-(4-methoxynaphthalen-1-yl)prop-2-enoate



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Specifications	Limits
Preferred IUPAC Name	ethyl (E)-3-(4-methoxynaphthalen-1-yl)prop-2-enoate
Systematic IUPAC Name	ethyl (E)-3-(4-methoxynaphthalen-1-yl)prop-2-enoate
Traditional IUPAC Name	(E)-3-(4-methoxy-1-naphthyl)acrylic acid ethyl ester
Standard InChI	InChI=1S/C16H16O3/c1-3-19-16(17)11-9-12-8-10-15(18-2)14-7-5-4-6-13(12)14/h4-11H,3H2,1-2H3/b11-9+
Standard InChIKey	VBZWLZWCHZBRPA-PKNCBQFBNSA-N
XLogP3-AA Log P	3.8
Exact Mass	256.109944368
Molecular Weight	256.30
Canonical SMILES	CCOC(=O)C=CC1=CC=C(C2=CC=CC=C12)OC
Isomeric SMILES	CCOC(=O)/C=C/C1=CC=C(C2=CC=CC=C12)OC

Specifications Limits

Polar Surface Area 35.5

Topological

Monoisotopic Weight 256.109944368

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