## 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 |

| 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-PKNBQFBNSA-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 |