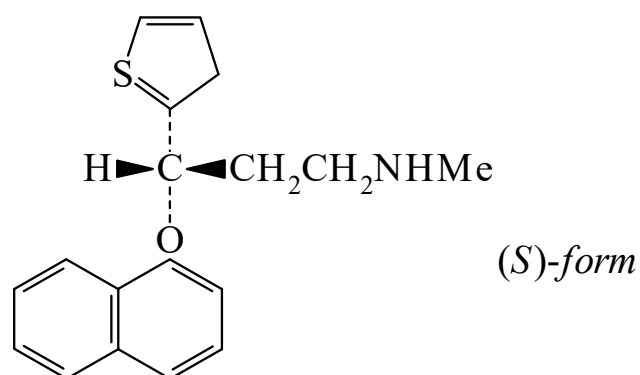




>>Entry Name: Duloxetine, INN

Synonym(s): *N*-Methyl- γ -(1-naphthalenyloxy)-2-thiophenepropanamine, 9Cl. *N*-Methyl-3-phenoxy-3-(2-thienyl)propylamine



Related CAS Registry Numbers(s): 116539-58-3 116539-60-7 116817-13-1 116817-77-7 116817-86-8 118625-29-9

Type of Compound Code(s): XA6801 XA4637 XA1450

Molecular Formula: C₁₈H₁₉NOS

Molecular Weight: 297.42

Accurate Mass: 297.118734

Percentage Composition: C 72.69%; H 6.44%; N 4.71%; O 5.38%; S 10.78%

Use/Importance: Inhibitor of 5-hydroxytryptamine and noradrenaline reuptake. Antidepressant

Calculated Log P Data: Log P 3.75 (uncertain value) (calc)

>>Variant: (*S*)-form

Synonym(s): LY248686

CAS Registry Number: 116539-59-4

Molecular Formula: C₁₈H₁₉NOS

Molecular Weight: 297.42

Accurate Mass: 297.118734

Percentage Composition: C 72.69%; H 6.44%; N 4.71%; O 5.38%; S 10.78%

>>Derivative: Hydrochloride

Synonym(s): Duloxetine hydrochloride, USAN

CAS Registry Number: 136434-34-9

>>Derivative: Maleate

Melting Point: Mp 118-122°

Optical Rotation: [α]_D +82. [α]_{Hg363} +391 (c, 1 in MeOH)

>>Derivative: Oxalate

CAS Registry Number: 116817-14-2

Physical Description: Cryst. (EtOAc/MeOH)

Melting Point: Mp 136-138.5°

References:

Eur. Pat., 1988, *Eli Lilly*, 273 658; *CA*, **109**, 170224n, (*synth, pharmacol*)

Wong, D.T. *et al.*, *Life Sci.*, 1988, **43**, 2049, (*pharmacol*)

Deeter, J. *et al.*, *Tet. Lett.*, 1990, **31**, 7101, (*synth, abs config*)

Wong, D.T. *et al.*, *Neuropsychopharmacology*, 1993, **8**, 23, (*pharmacol*)

Fuller, R.W. *et al.*, *J. Pharmacol. Exp. Ther.*, 1994, **269**, 132, (*pharmacol*)

Thor, K.B. *et al.*, *J. Pharmacol. Exp. Ther.*, 1995, **274**, 1014, (*pharmacol*)