

Noscapine

Other names:

(-)-Narcotine
(-)-«alpha»-Narcotine
(-)-Â«alphaÂ»-Narcotine
1(3H)-Isobenzofuranone,
6,7-dimethoxy-3-(5,6,7,8-tetrahydro-4-methoxy-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-yl)-
[S-(R*,S*)]-
Noscapal
Coscopin
Coscotabs
Hederix (free base)
Key-Tusscapine
L-«alpha»-Narcotine
L-Â«alphaÂ»-Narcotine
Longactin
Longatin
Lyobex
Methoxyhydrastine
NSC 5366
Narcompren
Narcosine
Narcotin
Narcotine
Narcotine alkaloid
Narcotussin
Narkotin
Nectadon
Nicolane
Nipaxon
Noscapal
Noscapalin
Noscapin
O-Methylnarcotoline
Opian
Opianin
Opianine
Phthalide,
6,7-dimethoxy-3-(5,6,7,8-tetrahydro-4-methoxy-6-methyl-1,3-dioxolo(4,5-g)isoquinolin-5-yl)-
Terbenol
Tusscapine
Vadebex
[S-(R*,S*)]-6,7-Dimethoxy-3-(5,6,7,8-tetrahydro-4-methoxy-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-5-yl)-
«alpha»-Narcotine
Â«alphaÂ»-Narcotine

Inchi: InChI=1S/C22H23NO7/c1-23-8-7-11-9-14-20(29-10-28-14)21(27-4)15(11)17(23)18-12-5
InchiKey: AKNNEGZIBPJZJG-ZWKOTPCHSA-N
Formula: C22H23NO7
SMILES: COc1ccc2c(c1OC)C(=O)OC2C1c2c(cc3c(c2OC)OCO3)CCN1C
Mol. weight [g/mol]: 413.42
CAS: 128-62-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Aqueous Solubility Prediction Method
logp	2.882		Crippen Method
mcvol	287.510	ml/mol	McGowan Method
rinpol	3170.00		NIST Webbook
rinpol	3168.00		NIST Webbook
rinpol	3135.00		NIST Webbook
rinpol	3145.00		NIST Webbook
rinpol	3110.00		NIST Webbook
rinpol	3168.00		NIST Webbook
rinpol	3117.00		NIST Webbook
rinpol	3120.00		NIST Webbook
rinpol	3170.00		NIST Webbook
rinpol	3145.00		NIST Webbook
rinpol	3154.00		NIST Webbook
rinpol	3170.00		NIST Webbook
rinpol	3146.00		NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C128621&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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