

SUFENTANIL

Other names:	N-[4-(Methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]propionalalide N-[4-(Methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidyl]propionanilide N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenylpropanamide (Sufentanil) Propanamide, N-[4-(methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidinyl]-N-phenyl- R-30730 Sufentanyl
Inchi:	InChI=1S/C22H30N2O2S/c1-3-21(25)24(19-8-5-4-6-9-19)22(18-26-2)12-15-23(16-13-22)
InchiKey:	GGCSSNBKKAUURC-UHFFFAOYSA-N
Formula:	C22H30N2O2S
SMILES:	CCC(=O)N(c1ccccc1)C1(COC)CCN(CCc2cccs2)CC1
Mol. weight [g/mol]:	386.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Aqueous Solubility Prediction Method
logp	4.215		Crippen Method
mcvol	310.510	ml/mol	McGowan Method
tf	389.90	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	23.85	kJ/mol	370.20	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56030547&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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