

Fentanyl

Other names:	1-(2-Phenylethyl)-4-(N-propananilido)piperidine 1-Phenethyl-4-(N-Phenylpropionamido)piperidine 1-Phenethyl-4-N-propionylanilinopiperidine Duragesic Fentanest Fentanil Fentora Matrifen N-(1-Phenylethyl-4-piperidiny)propionanilide N-Phenethyl-4-(N-propionylanilino)piperidine N-phenyl-N[1-(2-phenylethyl)-4-piperidiny]propanamide (fentanyl) Phentanyl Propanamide, N-phenyl-N-[1-(2-phenylethyl)-4-piperidiny]- Propionanilide, N-(1-phenethyl-4-piperidy)- R 4263 Sentonil Sublimase Sublimaze
Inchi:	InChI=1S/C22H28N2O/c1-2-22(25)24(20-11-7-4-8-12-20)21-14-17-23(18-15-21)16-13-19
InchiKey:	PJMPHNIQZUBGLI-UHFFFAOYSA-N
Formula:	C22H28N2O
SMILES:	CCC(=O)N(c1ccccc1)C1CCN(CCc2ccccc2)CC1
Mol. weight [g/mol]:	336.47
CAS:	437-38-7

Physical Properties

Property code	Value	Unit	Source
hfus	30.10	kJ/mol	Vapor Pressure and Enthalpy of Vaporization of Fentanyl
hsub	144.60 ± 7.20	kJ/mol	NIST Webbook
log10ws	-4.69		Crippen Method
logp	4.137		Crippen Method
mcvol	283.990	ml/mol	McGowan Method
rinpol	2730.00		NIST Webbook
rinpol	2718.00		NIST Webbook
rinpol	2730.00		NIST Webbook

rinpol	2757.00	NIST Webbook
rinpol	2720.00	NIST Webbook
rinpol	2718.00	NIST Webbook
rinpol	2720.00	NIST Webbook
rinpol	2681.00	NIST Webbook
rinpol	2701.00	NIST Webbook
rinpol	2701.00	NIST Webbook
rinpol	2725.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.10	kJ/mol	358.30	NIST Webbook
hfust	22.51	kJ/mol	357.20	NIST Webbook
hvapt	107.20 ± 4.20	kJ/mol	458.00	NIST Webbook

Sources

Vapor Pressure and Enthalpy of Vaporization of Fentanyl: McGowan Method:

<https://www.doi.org/10.1021/je7005067>

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C437387&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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