

Fenpropidin

Other names:	1-(3-(4-(1,1-dimethylethyl)phenyl)-2-methylpropyl)piperidine 1-(3-(4-(tert-butyl)phenyl)-2-methylpropyl)piperidine Fenpropidine Patrol Piperidine, 1-(3-(4-(1,1-dimethylethyl)phenyl)-2-methylpropyl)- Ro-12-3049
Inchi:	InChI=1S/C19H31N/c1-16(15-20-12-6-5-7-13-20)14-17-8-10-18(11-9-17)19(2,3)4/h8-11,
InchiKey:	MGNFYQILYYYUBS-UHFFFAOYSA-N
Formula:	C19H31N
SMILES:	CC(Cc1ccc(C(C)(C)C)cc1)CN1CCCCC1
Mol. weight [g/mol]:	273.46
CAS:	67306-00-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	4.649		Crippen Method
mcvol	253.930	ml/mol	McGowan Method
rinpol	1928.00		NIST Webbook
rinpol	1936.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	80.90	kJ/mol	298.00	The Vaporization Enthalpy and vapor Pressure of Fenpropidin and Phencyclidine (PCP) at T/K = 298.15 by Correlation Gas Chromatography

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67306007&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Vaporization Enthalpy and vapor Pressure of Fenpropidin and McGowan's Method (PCP) at T/K = 298.15 by Correlation Gas Chromatography:	https://www.doi.org/10.1021/acs.jced.5b00737 http://link.springer.com/article/10.1007/BF02311772

Legend

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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