Capsaicin

Other names:	(E)-N-(4-Hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide
	(E)-N-[(4-Hydroxy-3-methoxyphenyl)-methyl]-8-methyl-6-nonenamide
	6-Nonenamide, 8-methyl-N-vanillyl-, (E)-
	6-Nonenamide, N-[(4-hydroxy-3-methoxyphenyl)methyl]-8-methyl-, (E)-
	Adlea
	Axsain
	Capsaicine
	E-Capsaicin
	Mioton
	N-((4-Hydroxy-3-methoxyphenyl)methyl)-8-methyl-6-nonenamide
	N-(4-Hydroxy-3-methoxybenzyl)-8-methylnon-trans-6-enamide
	NCI-C56564
	Zostrix
	trans-8-Methyl-N-vanillyl-6-nonenamide
	trans-N-((4-Hydroxy-3-methoxyphenyl)methyl)-8-methyl-6-nonenamide
Inchi:	InChI=1S/C18H27NO3/c1-14(2)8-6-4-5-7-9-18(21)19-13-15-10-11-16(20)17(12-15)22-3/h
InchiKey:	YKPUWZUDDOIDPM-SOFGYWHQSA-N
Formula:	C18H27NO3
SMILES:	COc1cc(CN=C(O)CCCCC=CC(C)C)ccc1O
Mol. weight [g/mol]:	305.41
CAS:	404-86-4

Physical Properties

Property code	Value	Unit	Source
hf	-467.18	kJ/mol	Joback Method
hvap	93.67	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.630		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
tb	918.40	K	Joback Method
tc	1134.15	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C404864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Binary and Ternary Systems Containing Vanillin and Vanillic Acid in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.6b00322
Solubilities of Palmitic Acid + Capsaicin in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.7b00576
Solubilities of Binary Systems alpha-Tocopherol + Capsaicin and alpha-Tocopherol + Palmitic Acid in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.8b00996
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature