

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/
InchiKey:	YKPUWZUDDOIDPM-SOFGYWHQSA-N
Formula:	C18H27NO3
SMILES:	COc1cc(CN=C(O)CCCC=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

Solubilities of Palmitic Acid + Capsaicin in Supercritical Carbon Dioxide
Solubilities of Binary Systems
alpha-Tocopherol + Capsaicin and alpha-Tocopherol + Palmitic Acid in Supercritical Carbon Dioxide: McGowan Method:

<https://www.doi.org/10.1021/acs.jced.7b00576>

<https://www.doi.org/10.1021/acs.jced.8b00996>

https://en.wikipedia.org/wiki/Joback_method

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

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>

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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