Dihydrocapsaicin

Other names:	8-methyl-N-vanillylnonanamide
	N-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide
	Nonanamide, N-[(4-hydroxy-3-methoxyphenyl)methyl]-8-methyl-
Inchi:	InChI=1S/C18H29NO3/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:	XJQPQKLURWNAAH-UHFFFAOYSA-N
Formula:	C18H29NO3
SMILES:	COc1cc(CN=C(O)CCCCCCC(C)C)ccc1O
Mol. weight [g/mol]:	307.43
CAS:	19408-84-5

Physical Properties

Property code	Value	Unit	Source
hf	-584.40	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Measurement and Correlation for the Solubilities of Dihydrocapsaicin in n-Heptane, n-Hexane, n-Pentane, Ethyl Acetate, Acetone, Ethanol, and Water
hvap	93.71	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.854		Crippen Method
mcvol	264.010	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	2616.10		NIST Webbook
tb	914.24	K	Joback Method
tc	1126.42	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation for the Solubilities of Dihydrocapsaicin in n-Heptane, n-Hexane, n-Pentane, Ethyl Acetate, Acetone, Ethanol, and Water:	https://www.doi.org/10.1021/je1011136
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19408845&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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