Pipercallpsine

Other names: (2E,4E)-N-isobutyl-9-(3,4-methylenedioxyphenyl)nona-2,4-dienamide
(2E,4E)-9-(Benzo[d][1,3]dioxol-5-yl)-N-isobutylnona-2,4-dienamide
Inchi: InChI=1S/C20H27NO3/c1-16(2)14-21-20(22)10-8-6-4-3-5-7-9-17-11-12-18-19(13-17)24-
InchiKey: KXYVTCVLCVPQKR-ONNLMXTPSA-N
Formula: C20H27NO3
SMILES: CC(C)CN=C(O)C=CC=CCCCCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 329.43
CAS: 83029-39-4

Physical Properties

Property code	Value	Unit	Source
hf	-264.04	kJ/mol	Joback Method
hvap	92.56	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.853		Crippen Method
mcvol	272.730	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	2971.00		NIST Webbook
rinpol	2971.00		NIST Webbook
tb	935.57	K	Joback Method
tc	1155.24	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
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=C83029394&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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