N-Isobutyl-11-(3,4-methylenedioxyphenyl)-2E,4E,1 amide

Other names: (2E,4E,10E)-11-(Benzo[d][1,3]dioxol-5-yl)-N-isobutylundeca-2,4,10-trienamide

Inchi: InChI=1S/C22H29NO3/c1-18(2)16-23-22(24)12-10-8-6-4-3-5-7-9-11-19-13-14-20-21(15-

InchiKey: RPOYGOULCHMVBB-ADDDGJNWSA-N

Formula: C22H29NO3

SMILES: CC(C)CN=C(O)C=CC=CCCCCC=Cc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 355.47

CAS: 54794-74-0

Physical Properties

Property code	Value	Unit	Source
hf	-188.10	kJ/mol	Joback Method
hvap	96.97	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.714		Crippen Method
mcvol	296.610	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	2786.80		NIST Webbook
rinpol	2786.80		NIST Webbook
tb	985.49	K	Joback Method
tc	1211.44	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54794740&Units=SI

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

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