(2E,4E,12E)-13-(Benzo[d][1,3]dioxol-5-yl)-N-isobut

Inchi: InChI=1S/C24H33NO3/c1-20(2)18-25-24(26)14-12-10-8-6-4-3-5-7-9-11-13-21-15-16-22-
InchiKey: FPMPOFBEYSSYDQ-AUVZEZIHSA-N
Formula: C24H33NO3
SMILES: CC(C)CN=C(O)C=CC=CCCCCCCC=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 383.52
CAS: 55038-30-7

Physical Properties

Property code	Value	Unit	Source
hf	-229.38	kJ/mol	Joback Method
hvap	101.42	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.494		Crippen Method
mcvol	324.790	ml/mol	McGowan Method
pc	1172.83	kPa	Joback Method
rinpol	3481.00		NIST Webbook
rinpol	3481.00		NIST Webbook
tb	1031.25	K	Joback Method
tc	1263.15	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55038307&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

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