(2E,4E,8E)-9-(Benzo[d][1,3]dioxol-5-yl)-N-isobutyl

Inchi: InChI=1S/C20H25NO3/c1-16(2)14-21-20(22)10-8-6-4-3-5-7-9-17-11-12-18-19(13-17)24-
InchiKey: BPSWISYORIWKCT-FCGWLDPVSA-N
Formula: C20H25NO3
SMILES: CC(C)CN=C(O)C=CC=CCCC=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 327.42
CAS: 94079-67-1

Physical Properties

Property code	Value	Unit	Source
hf	-146.82	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.934		Crippen Method
mcvol	268.430	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	3063.50		NIST Webbook
rinpol	3063.50		NIST Webbook
tb	939.73	K	Joback Method
tc	1163.46	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=C94079671&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