Isophthalic acid, monoamide, N-butyl-, isohexyl ester

Inchi: InChI=1S/C18H27NO3/c1-4-5-11-19-17(20)15-9-6-10-16(13-15)18(21)22-12-7-8-14(2)3/h

InchiKey: IXGZPTZANLUORU-UHFFFAOYSA-N

Formula: C18H27NO3

SMILES: CCCCN=C(O)c1cccc(C(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
hf	-519.67	kJ/mol	Joback Method
hvap	87.44	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.384		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	887.49	K	Joback Method
tc	1095.76	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345811&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