Isophthalic acid, monoamide, N-(2-ethylhexyl)-, ethyl ester

Inchi:	InChI=1S/C18H27NO3/c1-4-7-9-14(5-2)13-19-17(20)15-10-8-11-16(12-15)18(21)22-6-3/I
InchiKey:	YRSQTDDUMGEGHQ-UHFFFAOYSA-N
Formula:	C18H27NO3
SMILES:	CCCCC(CC)CN=C(O)c1cccc(C(=O)OCC)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	2496.00		NIST Webbook
rinpol	2496.00		NIST Webbook
tb	887.49	K	Joback Method
tc	1095.76	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345833&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