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

Inchi: InChI=1S/C19H29NO3/c1-4-7-9-15(6-3)14-20-18(21)16-10-8-11-17(13-16)19(22)23-12-5

InchiKey: QVGYMELIPQEEGU-UHFFFAOYSA-N

Formula: C19H29NO3

SMILES: CCCCC(CC)CN=C(O)c1cccc(C(=O)OCCC)c1

Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
hf	-540.31	kJ/mol	Joback Method
hvap	89.67	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.774		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2598.00		NIST Webbook
rinpol	2598.00		NIST Webbook
tb	910.37	K	Joback Method
tc	1120.17	K	Joback Method

Sources

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=U345834&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

https://www.chemeo.com/cid/96-396-7/Isophthalic-acid-monoamide-N-2-ethylhexyl-propyl-ester.pdf

Generated by Cheméo on 2024-10-12 07:18:57.526117106 +0000 UTC m=+3298400.163086354.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.