Glutaric acid, monoamide, N-(2-biphenyl)-, decyl ester

Inchi: InChI=1S/C27H37NO3/c1-2-3-4-5-6-7-8-14-22-31-27(30)21-15-20-26(29)28-25-19-13-12

InchiKey: ZAYXCZMCRWVGDB-UHFFFAOYSA-N

Formula: C27H37NO3

SMILES: CCCCCCCCCCOC(=O)CCCC(O)=Nc1ccccc1-c1ccccc1

Mol. weight [g/mol]: 423.59

Physical Properties

Property code	Value	Unit	Source
hf	-463.62	kJ/mol	Joback Method
hvap	110.14	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	7.796		Crippen Method
mcvol	362.760	ml/mol	McGowan Method
pc	1024.00	kPa	Joback Method
rinpol	3386.00		NIST Webbook
rinpol	3386.00		NIST Webbook
tb	1120.53	K	Joback Method
tc	1374.70	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360048&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