3-Benzofurancarboxamide, n-cycloheptyl-2,3-dihydro-3-phenyl-

Inchi: InChI=1S/C22H25NO2/c24-21(23-18-12-6-1-2-7-13-18)22(17-10-4-3-5-11-17)16-25-20-1

InchiKey: FVXPYXMERWFKFZ-UHFFFAOYSA-N

Formula: C22H25NO2

SMILES: OC(=NC1CCCCCC1)C1(c2ccccc2)COc2ccccc21

Mol. weight [g/mol]: 335.44

CAS: 95133-29-2

Physical Properties

Property code	Value	Unit	Source
hf	-111.42	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.044		Crippen Method
mcvol	269.020	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
tb	987.59	K	Joback Method
tc	1247.35	K	Joback Method

Sources

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=C95133292&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature