

3-Benzofuran carboxamide, n-(n-butyl)-2,3-dihydro-3-phenyl-

Inchi: InChI=1S/C19H21NO2/c1-2-3-13-20-18(21)19(15-9-5-4-6-10-15)14-22-17-12-8-7-11-16(
InchiKey: HTEOHDFPZFBYES-UHFFFAOYSA-N
Formula: C19H21NO2
SMILES: CCCCNC(=O)C1(c2ccccc2)COc2ccccc21
Mol. weight [g/mol]: 295.38
CAS: 94310-89-1

Physical Properties

Property code	Value	Unit	Source
hf	-97.66	kJ/mol	Joback Method
hvap	86.45	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.122		Crippen Method
mcvol	237.610	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
tb	895.13	K	Joback Method
tc	1131.21	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C94310891&Units=SI>

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

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