

2-Phenyl-4-benz[d]oxazinone

Other names:	2-Phenyl-3,1-benzoxazinone-(4)
	2-Phenyl-4-[4H]-3,1-benzoxazinone
	2-phenyl-4H-3,1-benzoxazin-4-one
	3-Phenyl-1H-2,4-benzoxazin-1-one
	3-Phenyl-2,4-benzoxazin-1-one
	4H-3,1-benzoxazin-4-one, 2-phenyl-
	H-170
	Linarotox
	NSC 16082
Inchi:	bentranil
	linurotox
	InChI=1S/C14H9NO2/c16-14-11-8-4-5-9-12(11)15-13(17-14)10-6-2-1-3-7-10/h1-9H
	HTTLBYITFHMZYFK-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	O=c1oc(-c2ccccc2)nc2ccccc12
Mol. weight [g/mol]:	223.23

Physical Properties

Property code	Value	Unit	Source
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-4.61		Aqueous Solubility Prediction Method
logp	2.855		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
tb	664.22	K	Cheméo Relay (1.0)
tf	397.15	K	Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.70	K	1.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Solubility of Anti-Inflammatory,
Anti-Cancer, and Anti-HIV Drugs in
Supercritical Carbon Dioxide

<https://www.doi.org/10.1021/je049551l>

Supercritical Carbon Dioxide

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1022464&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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