Benzo(b)naphtho(1,2-d)furan

Other names:	NSC 109422
	«gamma»-Brazan
Inchi:	InChI=1S/C16H10O/c1-2-6-12-11(5-1)9-10-15-16(12)13-7-3-4-8-14(13)17-15/h1-10H
InchiKey:	XVWNNQQHTXDOLJ-UHFFFAOYSA-N
Formula:	C16H10O
SMILES:	c1ccc2c(c1)ccc1oc3ccccc3c12
Mol. weight [g/mol]:	218.25
CAS:	205-39-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.62		Crippen Method
logp	4.739		Crippen Method
mcvol	164.330	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	13.70	kJ/mol	315.90	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C205390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume