Benzo[b]naphtho[2,3-d]furan

Other names: Benzonaphthofuran
Inchi: InChI=1S/C16H10O/c1-2-6-12-10-16-14(9-11(12)5-1)13-7-3-4-8-15(13)17-16/h1-10H
InchiKey: FTMRMQALUDDFQO-UHFFFAOYSA-N
Formula: C16H10O
SMILES: c1ccc2cc3c(cc2c1)oc1ccccc13
Mol. weight [g/mol]: 218.25
CAS: 243-42-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.62		Crippen Method
logp	4.739		Crippen Method
mcvol	164.330	ml/mol	McGowan Method
rinpol	2089.00		NIST Webbook
rinpol	356.83		NIST Webbook
rinpol	353.60		NIST Webbook
rinpol	358.58		NIST Webbook
rinpol	354.30		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	353.47		NIST Webbook
rinpol	349.06		NIST Webbook
rinpol	354.09		NIST Webbook
rinpol	349.26		NIST Webbook
rinpol	354.37		NIST Webbook
rinpol	356.83		NIST Webbook
rinpol	353.47		NIST Webbook
tf	479.30 ± 1.00	K	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C243425&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point