Benzo[b]naphtho[2,1-d]furan

Other names: Benzo[b]naphtho[1,2-d]furan
Inchi: InChI=1S/C16H10O/c1-2-6-12-11(5-1)9-10-14-13-7-3-4-8-15(13)17-16(12)14/h1-10H
InchiKey: BCBSVZISIWCHFM-UHFFFAOYSA-N
Formula: C16H10O
SMILES: c1ccc2c(c1)ccc1c3ccccc3oc21
Mol. weight [g/mol]: 218.25
CAS: 239-30-5

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	354.52		NIST Webbook
rinpol	357.86		NIST Webbook
rinpol	355.65		NIST Webbook
rinpol	352.34		NIST Webbook
rinpol	355.65		NIST Webbook
rinpol	357.86		NIST Webbook
rinpol	345.10		NIST Webbook
rinpol	357.86		NIST Webbook
tb	662.00	K	NIST Webbook
tf	376.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.90	kJ/mol	373.70	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=C239305&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point