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]: 218.26

Physical Properties

Property code	Value	Unit	Source
hf	149.94	kJ/mol	Cheméo Relay (1.0)
hvap	100.26	kJ/mol	Cheméo Relay (1.0)
ie	7.62	eV	Cheméo Relay (1.0)
log10ws	-6.25		Cheméo Relay (1.0)
logp	4.739		Crippen Method
mcvol	164.330	ml/mol	McGowan Method
pc	2763.21	kPa	Cheméo Relay (1.0, beta)
tb	664.61	K	Cheméo Relay (1.0)
tc	970.29	K	Cheméo Relay (1.0)
tf	373.76	K	Cheméo Relay (1.0)
vc	0.642	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C205390&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume