DINAPHTHO[2,1-B:1',2'-D]FURAN

Inchi: InChI=1S/C20H12O/c1-3-7-15-13(5-1)9-11-17-19(15)20-16-8-4-2-6-14(16)10-12-18(20)2
InchiKey: QIMOZEUDRUTIBS-UHFFFAOYSA-N
Formula: C20H12O
SMILES: c1ccc2c(c1)ccc1oc3ccc4ccccc4c3c12
Mol. weight [g/mol]: 268.31

Physical Properties

Property code	Value	Unit	Source
af	0.6107		Cheméo Relay (1.0)
hf	230.39	kJ/mol	Cheméo Relay (1.0)
hvap	123.40	kJ/mol	Cheméo Relay (1.0)
ie	7.61	eV	Cheméo Relay (1.0)
log10ws	-7.79		Cheméo Relay (1.0)
logp	5.892		Crippen Method
mcvol	201.230	ml/mol	McGowan Method
pc	2124.37	kPa	Cheméo Relay (1.0, beta)
tb	748.99	K	Cheméo Relay (1.0)
tc	1072.89	K	Cheméo Relay (1.0)
tf	475.16	K	Cheméo Relay (1.0)
vc	0.781	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C194638&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

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
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