DINAPHTHO(1,2-B:2',1'-D)THIOPHENE

Other names: 1,2,7,8-Dibenzo-9-thiafluorene
Inchi: InChI=1S/C20H12S/c1-3-7-15-13(5-1)9-11-17-18-12-10-14-6-2-4-8-16(14)20(18)21-19(1
InchiKey: RHACEINAFSEPBJ-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)ccc1c3ccc4ccccc4c3sc21
Mol. weight [g/mol]: 284.38

Physical Properties

Property code	Value	Unit	Source
af	0.5691		Cheméo Relay (1.0)
hf	359.37	kJ/mol	Cheméo Relay (1.0)
hvap	127.17	kJ/mol	Cheméo Relay (1.0)
ie	7.40	eV	Cheméo Relay (1.0)
log10ws	-8.36		Cheméo Relay (1.0)
logp	6.361		Crippen Method
mcvol	211.710	ml/mol	McGowan Method
pc	2034.62	kPa	Cheméo Relay (1.0, beta)
rinpol	483.24		NIST Webbook
rinpol	482.60		NIST Webbook
tb	783.28	K	Cheméo Relay (1.0)
tc	1090.95	K	Cheméo Relay (1.0)
tf	495.36	K	Cheméo Relay (1.0)
vc	0.802	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C239725&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume