2,5-Diphenylfuran

Other names: 2,5-Diphenylfuran
PPF
Inchi: InChI=1S/C16H12O/c1-3-7-13(8-4-1)15-11-12-16(17-15)14-9-5-2-6-10-14/h1-12H
InchiKey: VUPDHIIPAKIKAB-UHFFFAOYSA-N
Formula: C16H12O
SMILES: c1ccc(-c2ccc(-c3ccccc3)o2)cc1
Mol. weight [g/mol]: 220.27

Physical Properties

Property code	Value	Unit	Source
af	0.4871		Cheméo Relay (1.0)
gf	239.33	kJ/mol	Cheméo Relay (1.0, beta)
hf	137.60	kJ/mol	Cheméo Relay (1.0)
hvap	93.35	kJ/mol	Cheméo Relay (1.0)
ie	8.25	eV	Cheméo Relay (1.0)
log10ws	-5.28		Cheméo Relay (1.0)
logp	4.614		Crippen Method
mcvol	175.190	ml/mol	McGowan Method
pc	3059.60	kPa	Cheméo Relay (1.0, beta)
tb	618.61	K	Cheméo Relay (1.0)
tc	876.01	K	Cheméo Relay (1.0)
tf	334.51	K	Cheméo Relay (1.0)
vc	0.675	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	102.00	kJ/mol	340.00	NIST Webbook

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C955839&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

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation 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