3-[Bis(4-methoxyphenyl)amino]-2-benzofuran-1(3

Inchi: InChI=1S/C22H19NO4/c1-25-17-11-7-15(8-12-17)23(16-9-13-18(26-2)14-10-16)21-19-5-

InchiKey: DZQHVCLQLIMOKX-UHFFFAOYSA-N

Formula: C22H19NO4

SMILES: COc1ccc(N(c2ccc(OC)cc2)C2OC(=O)c3ccccc32)cc1

Mol. weight [g/mol]: 361.39

CAS: 95166-04-4

Physical Properties

Property code	Value	Unit	Source
gf	195.52	kJ/mol	Joback Method
hf	-216.04	kJ/mol	Joback Method
hfus	44.71	kJ/mol	Joback Method
hvap	88.91	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.711		Crippen Method
mcvol	267.860	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
tb	956.53	K	Joback Method
tc	1213.60	K	Joback Method
tf	644.18	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.49	J/mol×K	956.53	Joback Method
cpg	862.87	J/mol×K	999.37	Joback Method
cpg	874.61	J/mol×K	1042.22	Joback Method
cpg	884.80	J/mol×K	1085.06	Joback Method
cpg	893.50	J/mol×K	1127.91	Joback Method
cpg	900.79	J/mol×K	1170.75	Joback Method
cpg	906.74	J/mol×K	1213.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95166044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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