3,3'(P-phenylene diimino) diphthalide

Inchi: InChI=1S/C22H16N2O4/c25-21-17-7-3-1-5-15(17)19(27-21)23-13-9-11-14(12-10-13)24-2
InchiKey: BINQLLJWERQNKD-UHFFFAOYSA-N
Formula: C22H16N2O4
SMILES: O=C1OC(Nc2ccc(NC3OC(=O)c4ccccc43)cc2)c2ccccc21
Mol. weight [g/mol]: 372.37
CAS: 102468-13-3

Physical Properties

Property code	Value	Unit	Source
gf	325.56	kJ/mol	Joback Method
hf	-109.09	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	103.59	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	4.249		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
tb	1101.10	K	Joback Method
tc	1380.48	K	Joback Method
tf	785.30	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.80	J/mol×K	1101.10	Joback Method
cpg	896.68	J/mol×K	1147.66	Joback Method
cpg	905.27	J/mol×K	1194.23	Joback Method
cpg	912.69	J/mol×K	1240.79	Joback Method
cpg	919.08	J/mol×K	1287.35	Joback Method
cpg	924.59	J/mol×K	1333.91	Joback Method
cpg	929.35	J/mol×K	1380.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102468133&Units=SI

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