[1,1'-Biphenyl]-4,4'-diamine, 2,2',3,3',5,5',6,6'-octafluoro-

Other names: Benzidine, 2,2',3,3',5,5',6,6'-octafluoro-
Octafluorobenzidine
2,2',3,3',5,5',6,6'-Octafluorobenzidine
4,4'-Biphenyldiamine, 2,2',3,3',5,5',6,6'-octafluoro-
4,4'-Diaminooctafluorodiphenyl
4,4'-Diaminooctafluorobiphenyl
Benzidine, octafluoro-
2,2',3,3',5,5',6,6'-Octafluoro[1,1'-biphenyl]-4,4'-diamine
octafluoro-4,4'-biphenylenediamine

Inchi: InChI=1S/C12H4F8N2/c13-3-1(4(14)8(18)11(21)7(3)17)2-5(15)9(19)12(22)10(20)6(2)16/

InchiKey: FWOLORXQTIGHFX-UHFFFAOYSA-N

Formula: C12H4F8N2

SMILES: Nc1c(F)c(F)c(-c2c(F)c(F)c(N)c(F)c2F)c(F)c1F

Mol. weight [g/mol]: 328.16

CAS: 1038-66-0

Physical Properties

Property code	Value	Unit	Source
gf	-1246.90	kJ/mol	Joback Method
hf	-1433.95	kJ/mol	Joback Method
hfus	46.06	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	3.631		Crippen Method
mcvol	166.540	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
tb	716.34	K	Joback Method
tc	910.56	K	Joback Method
tf	574.28	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	442.77	J/mol×K	716.34	Joback Method
cpg	451.18	J/mol×K	748.71	Joback Method
cpg	459.08	J/mol×K	781.08	Joback Method
cpg	466.49	J/mol×K	813.45	Joback Method
cpg	473.40	J/mol×K	845.82	Joback Method
cpg	479.81	J/mol×K	878.19	Joback Method
cpg	485.73	J/mol×K	910.56	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=C1038660&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