

4,4'-Dibromooctafluorobiphenyl

Other names:	Octafluoro-4,4'-dibromobiphenyl 1,1'-Biphenyl, 4,4'-dibromo-2,2',3,3',5,5',6,6'-octafluoro-4,4'-dibromo-2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl
Inchi:	InChI=1S/C12Br2F8/c13-3-9(19)5(15)1(6(16)10(3)20)2-7(17)11(21)4(14)12(22)8(2)18
InchiKey:	YXLMNFVUNLCJJY-UHFFFAOYSA-N
Formula:	C12Br2F8
SMILES:	Fc1c(F)c(-c2c(F)c(F)c(Br)c(F)c2F)c(F)c(F)c1Br
Mol. weight [g/mol]:	455.92
CAS:	10386-84-2

Physical Properties

Property code	Value	Unit	Source
gf	-1351.16	kJ/mol	Joback Method
hf	-1448.87	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	59.81	kJ/mol	Joback Method
log10ws	-9.05		Crippen Method
logp	5.991		Crippen Method
mcvol	181.580	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
tb	703.60	K	Joback Method
tc	903.69	K	Joback Method
tf	527.36	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.74	J/molxK	703.60	Joback Method
cpg	404.73	J/molxK	736.95	Joback Method
cpg	411.28	J/molxK	770.30	Joback Method
cpg	417.42	J/molxK	803.64	Joback Method
cpg	423.15	J/molxK	836.99	Joback Method
cpg	428.49	J/molxK	870.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C10386842&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/93-698-5/4-4-Dibromooctafluorobiphenyl.pdf>

Generated by Cheméo on 2024-05-01 09:11:54.4950388 +0000 UTC m=+16843963.415616115.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.