

O,o'-biphenol, 4,4'-difluoro-

Inchi:	InChI=1S/C12H8F2O2/c13-7-1-3-11(15)9(5-7)10-6-8(14)2-4-12(10)16/h1-6,15-16H
InchiKey:	PGTVKPNXXXWFMX-UHFFFAOYSA-N
Formula:	C12H8F2O2
SMILES:	Oc1ccc(F)cc1-c1cc(F)ccc1O
Mol. weight [g/mol]:	222.19
CAS:	388-69-2

Physical Properties

Property code	Value	Unit	Source
gf	-443.14	kJ/mol	Joback Method
hf	-587.73	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	72.58	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.043		Crippen Method
mcvol	147.700	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	697.06	K	Joback Method
tc	942.09	K	Joback Method
tf	527.50	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.51	J/molxK	697.06	Joback Method
cpg	396.76	J/molxK	737.90	Joback Method
cpg	406.36	J/molxK	778.74	Joback Method
cpg	415.47	J/molxK	819.57	Joback Method
cpg	424.28	J/molxK	860.41	Joback Method
cpg	432.93	J/molxK	901.25	Joback Method
cpg	441.60	J/molxK	942.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C388692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:

<https://www.chemeo.com/cid/115-191-2/O-o-biphenol-4-4-difluoro.pdf>

Generated by Cheméo on 2024-04-28 18:11:24.943337601 +0000 UTC m=+16617133.863914916.

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