

1,1'-Biphenyl-3-ol, 2',6,6'-trichloro

Inchi:	InChI=1S/C12H7Cl3O/c13-9-5-4-7(16)6-8(9)12-10(14)2-1-3-11(12)15/h1-6,16H
InchiKey:	OGWBKKTZNFSXEC-UHFFFAOYSA-N
Formula:	C12H7Cl3O
SMILES:	Oc1ccc(Cl)c(-c2c(Cl)cccc2Cl)c1
Mol. weight [g/mol]:	273.54

Physical Properties

Property code	Value	Unit	Source
gf	55.68	kJ/mol	Joback Method
hf	-76.89	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	75.01	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.019		Crippen Method
mcvol	175.010	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	1980.00		NIST Webbook
tb	735.17	K	Joback Method
tc	1004.96	K	Joback Method
tf	516.88	K	Joback Method
vc	0.605	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.99	J/mol×K	735.17	Joback Method
cpg	398.89	J/mol×K	780.13	Joback Method
cpg	408.05	J/mol×K	825.10	Joback Method
cpg	416.63	J/mol×K	870.06	Joback Method
cpg	424.77	J/mol×K	915.03	Joback Method
cpg	432.62	J/mol×K	959.99	Joback Method
cpg	440.33	J/mol×K	1004.96	Joback Method
dvisc	0.0001819	Paxs	516.88	Joback Method
dvisc	0.0001042	Paxs	553.26	Joback Method

dvisc	0.0000639	Paxs	589.64	Joback Method
dvisc	0.0000415	Paxs	626.03	Joback Method
dvisc	0.0000283	Paxs	662.41	Joback Method
dvisc	0.0000200	Paxs	698.79	Joback Method
dvisc	0.0000147	Paxs	735.17	Joback Method

Sources

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=R343516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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