

1,1'-Biphenyl-3-ol, 2,2',5-trichloro

Inchi:	InChI=1S/C12H7Cl3O/c13-7-5-9(12(15)11(16)6-7)8-3-1-2-4-10(8)14/h1-6,16H
InchiKey:	MPWBJAGTWICCSA-UHFFFAOYSA-N
Formula:	C12H7Cl3O
SMILES:	Oc1cc(Cl)cc(-c2ccccc2Cl)c1Cl
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
mvol	175.010	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		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/molxK	735.17	Joback Method
cpg	398.89	J/molxK	780.13	Joback Method
cpg	408.05	J/molxK	825.10	Joback Method
cpg	416.63	J/molxK	870.06	Joback Method
cpg	424.77	J/molxK	915.03	Joback Method
cpg	432.62	J/molxK	959.99	Joback Method
cpg	440.33	J/molxK	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

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=R343576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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