1,1'-Biphenyl-3-ol, 4',5,6-trichloro

Inchi: InChI=1S/C12H7Cl3O/c13-8-3-1-7(2-4-8)10-5-9(16)6-11(14)12(10)15/h1-6,16H
InchiKey: JQHGAFGNUUTSOY-UHFFFAOYSA-N
Formula: C12H7Cl3O
SMILES: Oc1cc(Cl)c(Cl)c(-c2ccc(Cl)cc2)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	2071.00		NIST Webbook
tb	735.17	K	Joback Method
tc	1004.96	K	Joback Method
tf	516.88	K	Joback Method
vc	0.605	m3/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	Pa×s	516.88	Joback Method
dvisc	0.0001042	Pa×s	553.26	Joback Method

dvisc	0.0000639	Pa×s	589.64	Joback Method
dvisc	0.0000415	Pa×s	626.03	Joback Method
dvisc	0.0000283	Pa×s	662.41	Joback Method
dvisc	0.0000200	Pa×s	698.79	Joback Method
dvisc	0.0000147	Pa×s	735.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R343709&Units=SI
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

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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