1,1'-Biphenyl-4-ol, 3,3'-dichloro

Inchi: InChI=1S/C12H8Cl2O/c13-10-3-1-2-8(6-10)9-4-5-12(15)11(14)7-9/h1-7,15H
InchiKey: JOHAARQQFBMIOV-UHFFFAOYSA-N
Formula: C12H8Cl2O
SMILES: Oc1ccc(-c2cccc(Cl)c2)cc1Cl
Mol. weight [g/mol]: 239.10

Physical Properties

Property code	Value	Unit	Source
gf	77.24	kJ/mol	Joback Method
hf	-49.68	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.366		Crippen Method
mcvol	162.770	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1929.00		NIST Webbook
tb	692.76	K	Joback Method
tc	960.07	K	Joback Method
tf	474.44	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.08	J/mol×K	692.76	Joback Method
cpg	419.03	J/mol×K	915.52	Joback Method
cpg	410.63	J/mol×K	870.97	Joback Method
cpg	401.79	J/mol×K	826.42	Joback Method
cpg	392.36	J/mol×K	781.86	Joback Method
cpg	382.17	J/mol×K	737.31	Joback Method
cpg	427.12	J/mol×K	960.07	Joback Method
dvisc	0.0000190	Pa×s	692.76	Joback Method
dvisc	0.0000267	Pa×s	656.37	Joback Method

dvisc	0.0000391	Pa×s	619.99	Joback Method
dvisc	0.0000600	Pa×s	583.60	Joback Method
dvisc	0.0000975	Pa×s	547.21	Joback Method
dvisc	0.0001697	Pa×s	510.83	Joback Method
dvisc	0.0003217	Pa×s	474.44	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=R344004&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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