

1,1'-Biphenyl, 3-chloro-4-methoxy-

Other names:	Anisole, 2-chloro-4-phenyl- 2-Chloro-4-phenylanisole
Inchi:	InChI=1S/C13H11ClO/c1-15-13-8-7-11(9-12(13)14)10-5-3-2-4-6-10/h2-9H,1H3
InchiKey:	SLBYCCHSURAIK-UHFFFAOYSA-N
Formula:	C13H11ClO
SMILES:	COc1ccc(-c2ccccc2)cc1Cl
Mol. weight [g/mol]:	218.68
CAS:	21424-83-9

Physical Properties

Property code	Value	Unit	Source
gf	147.21	kJ/mol	Joback Method
hf	-9.49	kJ/mol	Joback Method
hfus	22.12	kJ/mol	Joback Method
hvap	57.20	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.016		Crippen Method
mvol	164.620	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	620.01	K	Joback Method
tc	866.55	K	Joback Method
tf	366.30	K	Joback Method
vc	0.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.99	J/molxK	620.01	Joback Method
cpg	389.77	J/molxK	661.10	Joback Method
cpg	403.46	J/molxK	702.19	Joback Method
cpg	416.09	J/molxK	743.28	Joback Method
cpg	427.71	J/molxK	784.37	Joback Method
cpg	438.35	J/molxK	825.46	Joback Method
cpg	448.06	J/molxK	866.55	Joback Method

dvisc	0.0011043	Paxs	366.30	Joback Method
dvisc	0.0006656	Paxs	408.59	Joback Method
dvisc	0.0004411	Paxs	450.87	Joback Method
dvisc	0.0003137	Paxs	493.15	Joback Method
dvisc	0.0002354	Paxs	535.44	Joback Method
dvisc	0.0001843	Paxs	577.73	Joback Method
dvisc	0.0001491	Paxs	620.01	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=C21424839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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