4-CHLORODIPHENYLMETHANE

Other names:	p-Chlorobenzylbenzene
	p-Chlorodiphenylmethane
	Benzene, 1-chloro-4-(phenylmethyl)-
	Methane, (p-chlorophenyl)phenyl-
	4-Chlorodiphenylmethane
	Diphenylmethane, 4-chloro
Inchi:	InChI=1S/C13H11Cl/c14-13-8-6-12(7-9-13)10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey:	NPOGRKGIBGKRNI-UHFFFAOYSA-N
Formula:	C13H11Cl
SMILES:	Clc1ccc(Cc2ccccc2)cc1
Mol. weight [g/mol]:	202.68

Physical Properties

Property code	Value	Unit	Source
af	0.4227		Cheméo Relay (1.0)
gf	261.84	kJ/mol	Joback Method
hf	156.05	kJ/mol	Cheméo Relay (1.0)
hfus	21.32	kJ/mol	Joback Method
hvap	75.37	kJ/mol	Cheméo Relay (1.0)
ie	8.73	eV	Cheméo Relay (1.0)
log10ws	-4.86		Cheméo Relay (1.0)
logp	3.931		Crippen Method
mcvol	158.750	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	276.90		NIST Webbook
rinpol	276.90		NIST Webbook
tb	579.95	K	Cheméo Relay (1.0)
tc	801.11	K	Cheméo Relay (1.0)
tf	300.58	K	Cheméo Relay (1.0)
vc	0.590	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	351.47	J/mol×K	592.61	Joback Method
cpg	427.26	J/mol×K	842.20	Joback Method
cpg	417.22	J/mol×K	800.61	Joback Method
cpg	406.25	J/mol×K	759.01	Joback Method
cpg	394.27	J/mol×K	717.41	Joback Method
cpg	381.19	J/mol×K	675.81	Joback Method
cpg	366.95	J/mol×K	634.21	Joback Method
dvisc	0.0004265	Pa×s	462.08	Joback Method
dvisc	0.0001877	Pa×s	592.61	Joback Method
dvisc	0.0002363	Pa×s	549.10	Joback Method
dvisc	0.0003095	Pa×s	505.59	Joback Method
dvisc	0.0018486	Pa×s	331.55	Joback Method
dvisc	0.0006282	Pa×s	418.57	Joback Method
dvisc	0.0010122	Pa×s	375.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C831812&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
ie: Ionization energy
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