Bibenzyl, 3-chloro-

Other names:	1-Chloro-3-(2-phenylethyl)benzene
	1-(3-Chlorophenyl)-2-phenylethane
Inchi:	InChI=1S/C14H13Cl/c15-14-8-4-7-13(11-14)10-9-12-5-2-1-3-6-12/h1-8,11H,9-10H2
InchiKey:	NWVGKFZMBBPAJL-UHFFFAOYSA-N
Formula:	C14H13Cl
SMILES:	Clc1cccc(CCc2ccccc2)c1
Mol. weight [g/mol]:	216.71
CAS:	34176-92-6

Physical Properties

Property code	Value	Unit	Source
gf	270.26	kJ/mol	Joback Method
hf	113.56	kJ/mol	Joback Method
hfus	23.91	kJ/mol	Joback Method
hvap	56.36	kJ/mol	Joback Method
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-4.57		Crippen Method
logp	4.125		Crippen Method
mcvol	172.840	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	615.49	K	Joback Method
tc	859.62	K	Joback Method
tf	342.82	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.87	J/mol×K	615.49	Joback Method
cpg	415.99	J/mol×K	656.18	Joback Method
cpg	430.85	J/mol×K	696.87	Joback Method
cpg	444.54	J/mol×K	737.56	Joback Method
cpg	457.13	J/mol×K	778.25	Joback Method
cpg	468.70	J/mol×K	818.93	Joback Method

cpg	479.32	J/mol×K	859.62	Joback Method
dvisc	0.0017974	Pa×s	342.82	Joback Method
dvisc	0.0009670	Pa×s	388.26	Joback Method
dvisc	0.0005924	Pa×s	433.71	Joback Method
dvisc	0.0003983	Pa×s	479.15	Joback Method
dvisc	0.0002869	Pa×s	524.60	Joback Method
dvisc	0.0002177	Pa×s	570.04	Joback Method
dvisc	0.0001721	Pa×s	615.49	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=C34176926&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
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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