(4-Chlorobutyl)benzene

Other names:	1-Chloro-4-phenylbutane
	4-Phenyl-n-butyl chloride
	4-Phenylbutyl chloride
Inchi:	InChI=1S/C10H13Cl/c11-9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9H2
InchiKey:	FLLZCZIHURYEQP-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	ClCCCCc1ccccc1
Mol. weight [g/mol]:	168.67
CAS:	4830-93-7

Physical Properties

Property code	Value	Unit	Source
af	0.4435		Cheméo Relay (1.0)
gf	133.80	kJ/mol	Joback Method
hf	-32.75	kJ/mol	Cheméo Relay (1.0)
hfus	19.89	kJ/mol	Joback Method
hvap	61.35	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	Cheméo Relay (1.0)
log10ws	-3.78		Cheméo Relay (1.0)
logp	3.248		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
tb	508.40	K	Cheméo Relay (1.0)
tc	726.48	K	Cheméo Relay (1.0)
tf	229.30	K	Cheméo Relay (1.0)
vc	0.513	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.25	J/mol×K	492.31	Joback Method
cpg	299.62	J/mol×K	527.40	Joback Method

cpg	313.14	J/mol×K	562.49	Joback Method
cpg	325.84	J/mol×K	597.58	Joback Method
cpg	337.77	J/mol×K	632.66	Joback Method
cpg	348.95	J/mol×K	667.75	Joback Method
cpg	359.42	J/mol×K	702.84	Joback Method
dvisc	0.0035067	Pa×s	258.80	Joback Method
dvisc	0.0016801	Pa×s	297.72	Joback Method
dvisc	0.0009542	Pa×s	336.64	Joback Method
dvisc	0.0006094	Pa×s	375.56	Joback Method
dvisc	0.0004234	Pa×s	414.47	Joback Method
dvisc	0.0003131	Pa×s	453.39	Joback Method
dvisc	0.0002429	Pa×s	492.31	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28852e+01
Coeff. B	-3.58745e+03
Coeff. C	-7.74460e+01
Temperature range (K), min.	362.22
Temperature range (K), max.	551.12

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4830937&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume