4-n-Butylchlorobenzene

Other names:	Benzene, 1-butyl-4-chloro
	p-Clorobutylbenzene
	1-(4-chlorophenyl)butane
Inchi:	InChI=1S/C10H13Cl/c1-2-3-4-9-5-7-10(11)8-6-9/h5-8H,2-4H2,1H3
InchiKey:	SKNUPXIXICTRJE-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	CCCCc1ccc(Cl)cc1
Mol. weight [g/mol]:	168.66
CAS:	15499-27-1

Physical Properties

Property code	Value	Unit	Source
gf	124.17	kJ/mol	Joback Method
hf	-40.41	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	45.18	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.683		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
ripol	1641.00		NIST Webbook
ripol	1641.00		NIST Webbook
tb	497.29	K	Joback Method
tc	709.05	K	Joback Method
tf	271.32	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.58	J/mol×K	497.29	Joback Method
cpg	299.55	J/mol×K	532.58	Joback Method
cpg	312.73	J/mol×K	567.88	Joback Method
cpg	325.15	J/mol×K	603.17	Joback Method

cpg	336.84	J/mol×K	638.47	Joback Method
cpg	347.83	J/mol×K	673.76	Joback Method
cpg	358.16	J/mol×K	709.05	Joback Method
dvisc	0.0024596	Pa×s	271.32	Joback Method
dvisc	0.0013081	Pa×s	308.98	Joback Method
dvisc	0.0007980	Pa×s	346.64	Joback Method
dvisc	0.0005363	Pa×s	384.30	Joback Method
dvisc	0.0003870	Pa×s	421.97	Joback Method
dvisc	0.0002945	Pa×s	459.63	Joback Method
dvisc	0.0002336	Pa×s	497.29	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C15499271&Units=SI

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

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