

Benzene, (3-chlorobutyl)

Inchi:	InChI=1S/C10H13Cl/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6,9H,7-8H2,1H3
InchiKey:	MPRASCUUHIQYFQ-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	CC(Cl)CCc1ccccc1
Mol. weight [g/mol]:	168.66

Physical Properties

Property code	Value	Unit	Source
gf	131.36	kJ/mol	Joback Method
hf	-34.22	kJ/mol	Joback Method
hfus	16.37	kJ/mol	Joback Method
hvap	44.13	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.246		Crippen Method
mvol	140.240	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1240.00		NIST Webbook
tb	491.87	K	Joback Method
tc	707.30	K	Joback Method
tf	243.80	K	Joback Method
vc	0.530	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.46	J/molxK	491.87	Joback Method
cpg	300.25	J/molxK	527.77	Joback Method
cpg	314.13	J/molxK	563.68	Joback Method
cpg	327.16	J/molxK	599.58	Joback Method
cpg	339.35	J/molxK	635.49	Joback Method
cpg	350.77	J/molxK	671.39	Joback Method
cpg	361.43	J/molxK	707.30	Joback Method
dvisc	0.0050638	Paxs	243.80	Joback Method
dvisc	0.0020818	Paxs	285.14	Joback Method

dvisc	0.0010719	Paxs	326.49	Joback Method
dvisc	0.0006408	Paxs	367.84	Joback Method
dvisc	0.0004250	Paxs	409.18	Joback Method
dvisc	0.0003040	Paxs	450.52	Joback Method
dvisc	0.0002300	Paxs	491.87	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=R132133&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
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

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<https://www.chemeo.com/cid/18-886-9/Benzene-3-chlorobutyl.pdf>

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