

Benzene, [1-chloro-4-(3-methylbutyl)]

Inchi:	InChI=1S/C11H15Cl/c1-9(2)3-4-10-5-7-11(12)8-6-10/h5-9H,3-4H2,1-2H3
InchiKey:	XZUSXWMBZDIECA-UHFFFAOYSA-N
Formula:	C11H15Cl
SMILES:	CC(C)CCc1ccc(Cl)cc1
Mol. weight [g/mol]:	182.69

Physical Properties

Property code	Value	Unit	Source
gf	130.15	kJ/mol	Joback Method
hf	-66.33	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	47.02	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.929		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinsol	1303.00		NIST Webbook
tb	519.73	K	Joback Method
tc	732.95	K	Joback Method
tf	267.59	K	Joback Method
vc	0.587	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.45	J/molxK	519.73	Joback Method
cpg	398.47	J/molxK	697.42	Joback Method
cpg	386.48	J/molxK	661.88	Joback Method
cpg	373.73	J/molxK	626.34	Joback Method
cpg	360.16	J/molxK	590.80	Joback Method
cpg	345.74	J/molxK	555.27	Joback Method
cpg	409.71	J/molxK	732.95	Joback Method
dvisc	0.0002070	Paxs	519.73	Joback Method
dvisc	0.0002685	Paxs	477.71	Joback Method

dvisc	0.0003662	Paxs	435.68	Joback Method
dvisc	0.0005338	Paxs	393.66	Joback Method
dvisc	0.0008513	Paxs	351.64	Joback Method
dvisc	0.0015410	Paxs	309.61	Joback Method
dvisc	0.0033612	Paxs	267.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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