

Benzene, (1-chloro-3-methylbutyl)

Inchi:	InChI=1S/C11H15Cl/c1-9(2)8-11(12)10-6-4-3-5-7-10/h3-7,9,11H,8H2,1-2H3
InchiKey:	RROHTIQSMOHDLW-UHFFFAOYSA-N
Formula:	C11H15Cl
SMILES:	CC(C)CC(Cl)c1ccccc1
Mol. weight [g/mol]:	182.69

Physical Properties

Property code	Value	Unit	Source
gf	137.34	kJ/mol	Joback Method
hf	-60.14	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	45.97	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	4.013		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinsol	1279.00		NIST Webbook
tb	514.31	K	Joback Method
tc	731.21	K	Joback Method
tf	240.07	K	Joback Method
vc	0.581	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.44	J/molxK	514.31	Joback Method
cpg	401.43	J/molxK	695.06	Joback Method
cpg	389.04	J/molxK	658.91	Joback Method
cpg	375.79	J/molxK	622.76	Joback Method
cpg	361.64	J/molxK	586.61	Joback Method
cpg	346.53	J/molxK	550.46	Joback Method
cpg	413.00	J/molxK	731.21	Joback Method
dvisc	0.0002021	Paxs	514.31	Joback Method
dvisc	0.0002752	Paxs	468.60	Joback Method

dvisc	0.0004005	Paxs	422.90	Joback Method
dvisc	0.0006382	Paxs	377.19	Joback Method
dvisc	0.0011567	Paxs	331.48	Joback Method
dvisc	0.0025354	Paxs	285.78	Joback Method
dvisc	0.0074933	Paxs	240.07	Joback Method

Sources

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=R131789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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