Benzene, (3-chloro-3-methylbutyl)-

Inchi: InChI=1S/C11H15Cl/c1-11(2,12)9-8-10-6-4-3-5-7-10/h3-7H,8-9H2,1-2H3
InchiKey: GCAZETCXAVCJCN-UHFFFAOYSA-N
Formula: C11H15Cl
SMILES: CC(C)(Cl)CCc1ccccc1
Mol. weight [g/mol]: 182.69
CAS: 4830-95-9

Physical Properties

Property code	Value	Unit	Source
gf	145.06	kJ/mol	Joback Method
hf	-58.33	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	45.45	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.637		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1326.00		NIST Webbook
rinpol	1326.00		NIST Webbook
tb	511.96	K	Joback Method
tc	732.97	K	Joback Method
tf	272.49	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.04	J/mol×K	511.96	Joback Method
cpg	349.50	J/mol×K	548.80	Joback Method
cpg	364.81	J/mol×K	585.63	Joback Method
cpg	379.03	J/mol×K	622.47	Joback Method
cpg	392.23	J/mol×K	659.30	Joback Method
cpg	404.48	J/mol×K	696.14	Joback Method
cpg	415.84	J/mol×K	732.97	Joback Method

dvisc	0.0046976	Pa×s	272.49	Joback Method
dvisc	0.0020281	Pa×s	312.40	Joback Method
dvisc	0.0010592	Pa×s	352.31	Joback Method
dvisc	0.0006313	Pa×s	392.23	Joback Method
dvisc	0.0004140	Pa×s	432.14	Joback Method
dvisc	0.0002916	Pa×s	472.05	Joback Method
dvisc	0.0002169	Pa×s	511.96	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=C4830959&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
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