

Benzene, 3-chloro-1-methyl-4-(1-methylethenyl)

Inchi:	InChI=1S/C10H11Cl/c1-7(2)9-5-4-8(3)6-10(9)11/h4-6H,1H2,2-3H3
InchiKey:	SIZLKNFNLHRNGT-UHFFFAOYSA-N
Formula:	C10H11Cl
SMILES:	C=C(C)c1ccc(C)cc1Cl
Mol. weight [g/mol]:	166.65

Physical Properties

Property code	Value	Unit	Source
gf	193.83	kJ/mol	Joback Method
hf	63.76	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	45.25	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.682		Crippen Method
mvol	135.940	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1189.00		NIST Webbook
tb	498.83	K	Joback Method
tc	720.87	K	Joback Method
tf	268.12	K	Joback Method
vc	0.518	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.83	J/mol×K	498.83	Joback Method
cpg	280.90	J/mol×K	535.84	Joback Method
cpg	293.21	J/mol×K	572.84	Joback Method
cpg	304.77	J/mol×K	609.85	Joback Method
cpg	315.62	J/mol×K	646.86	Joback Method
cpg	325.79	J/mol×K	683.86	Joback Method
cpg	335.33	J/mol×K	720.87	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=R132113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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