

Benzene, 1-methyl-4-(2-chloro-1-methylethyl)

Inchi:	InChI=1S/C10H13Cl/c1-8-3-5-10(6-4-8)9(2)7-11/h3-6,9H,7H2,1-2H3
InchiKey:	SUXIXPCBVLIGFT-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	Cc1ccc(C(C)CCl)cc1
Mol. weight [g/mol]:	168.66

Physical Properties

Property code	Value	Unit	Source
gf	121.73	kJ/mol	Joback Method
hf	-45.69	kJ/mol	Joback Method
hfus	15.98	kJ/mol	Joback Method
hvap	44.79	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.337		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinsol	1258.00		NIST Webbook
tb	496.85	K	Joback Method
tc	713.53	K	Joback Method
tf	256.32	K	Joback Method
vc	0.530	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.81	J/mol×K	496.85	Joback Method
cpg	349.64	J/mol×K	677.42	Joback Method
cpg	338.41	J/mol×K	641.30	Joback Method
cpg	326.45	J/mol×K	605.19	Joback Method
cpg	313.72	J/mol×K	569.08	Joback Method
cpg	300.18	J/mol×K	532.96	Joback Method
cpg	360.16	J/mol×K	713.53	Joback Method
dvisc	0.0002211	Paxs	496.85	Joback Method
dvisc	0.0002853	Paxs	456.76	Joback Method

dvisc	0.0003866	Paxs	416.67	Joback Method
dvisc	0.0005590	Paxs	376.58	Joback Method
dvisc	0.0008825	Paxs	336.50	Joback Method
dvisc	0.0015764	Paxs	296.41	Joback Method
dvisc	0.0033760	Paxs	256.32	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=R131898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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