

Benzene, 1-chloro-2,3-dimethyl-

Inchi:	InChI=1S/C8H9Cl/c1-6-4-3-5-8(9)7(6)2/h3-5H,1-2H3
InchiKey:	NVLHGZIXTRYOKT-UHFFFAOYSA-N
Formula:	C8H9Cl
SMILES:	Cc1cccc(Cl)c1C
Mol. weight [g/mol]:	140.61
CAS:	608-23-1

Physical Properties

Property code	Value	Unit	Source
gf	97.70	kJ/mol	Joback Method
hf	-10.60	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	41.39	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.957		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1119.00		NIST Webbook
tb	456.51	K	Joback Method
tc	676.11	K	Joback Method
tf	261.30	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.65	J/molxK	456.51	Joback Method
cpg	213.88	J/molxK	493.11	Joback Method
cpg	224.50	J/molxK	529.71	Joback Method
cpg	234.54	J/molxK	566.31	Joback Method
cpg	244.00	J/molxK	602.91	Joback Method
cpg	252.92	J/molxK	639.51	Joback Method

cpg	261.31	J/molxK	676.11	Joback Method
dvisc	0.0016353	Paxs	261.30	Joback Method
dvisc	0.0009978	Paxs	293.84	Joback Method
dvisc	0.0006718	Paxs	326.37	Joback Method
dvisc	0.0004860	Paxs	358.90	Joback Method
dvisc	0.0003710	Paxs	391.44	Joback Method
dvisc	0.0002952	Paxs	423.98	Joback Method
dvisc	0.0002426	Paxs	456.51	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C608231&Units=SI

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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