

Benzene, 1,3-dichloro-4,6-dimethyl

Inchi:	InChI=1S/C8H8Cl2/c1-5-3-6(2)8(10)4-7(5)9/h3-4H,1-2H3
InchiKey:	SFPXVPWDXSCTBK-UHFFFAOYSA-N
Formula:	C8H8Cl2
SMILES:	Cc1cc(C)c(Cl)cc1Cl
Mol. weight [g/mol]:	175.06

Physical Properties

Property code	Value	Unit	Source
gf	76.14	kJ/mol	Joback Method
hf	-37.81	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	46.43	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.610		Crippen Method
mcvol	124.300	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1218.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1218.00		NIST Webbook
tb	498.92	K	Joback Method
tc	725.78	K	Joback Method
tf	303.74	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.14	J/molxK	498.92	Joback Method
cpg	271.75	J/molxK	687.97	Joback Method
cpg	263.69	J/molxK	650.16	Joback Method
cpg	255.11	J/molxK	612.35	Joback Method
cpg	246.01	J/molxK	574.54	Joback Method
cpg	236.36	J/molxK	536.73	Joback Method
cpg	279.32	J/molxK	725.78	Joback Method

dvisc	0.0002532	Paxs	498.92	Joback Method
dvisc	0.0003031	Paxs	466.39	Joback Method
dvisc	0.0003727	Paxs	433.86	Joback Method
dvisc	0.0004739	Paxs	401.33	Joback Method
dvisc	0.0006287	Paxs	368.80	Joback Method
dvisc	0.0008809	Paxs	336.27	Joback Method
dvisc	0.0013268	Paxs	303.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R528599&Units=SI
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

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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