

p-Toluic acid, 3-chloro-

Other names:	3-Chloro-4-methylbenzoic acid 3-Chloro-p-toluic acid Benzoic acid, 3-chloro-4-methyl-
Inchi:	InChI=1S/C8H7ClO2/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4H,1H3,(H,10,11)
InchiKey:	SDKUOEOJAXGCLU-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	Cc1ccc(C(=O)O)cc1Cl
Mol. weight [g/mol]:	170.59
CAS:	5162-82-3

Physical Properties

Property code	Value	Unit	Source
gf	-168.04	kJ/mol	Joback Method
hf	-275.41	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.347		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	602.56	K	Joback Method
tc	814.98	K	Joback Method
tf	372.05	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.09	J/molxK	602.56	Joback Method
cpg	264.46	J/molxK	637.96	Joback Method
cpg	272.30	J/molxK	673.37	Joback Method
cpg	279.65	J/molxK	708.77	Joback Method
cpg	286.51	J/molxK	744.17	Joback Method
cpg	292.91	J/molxK	779.58	Joback Method

cpg	298.86	J/mol×K	814.98	Joback Method
dvisc	0.0025922	Paxs	372.05	Joback Method
dvisc	0.0011790	Paxs	410.47	Joback Method
dvisc	0.0006137	Paxs	448.89	Joback Method
dvisc	0.0003540	Paxs	487.30	Joback Method
dvisc	0.0002214	Paxs	525.72	Joback Method
dvisc	0.0001475	Paxs	564.14	Joback Method
dvisc	0.0001036	Paxs	602.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5162823&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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