

4-(Chloromethyl)benzoic acid

Other names:	«alpha»-Chloro-p-toluylic acid Benzoic acid, 4-(chloromethyl)-
Inchi:	InChI=1S/C8H7ClO2/c9-5-6-1-3-7(4-2-6)8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	OITNBHJJGMFBN-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	O=C(O)c1ccc(CCl)cc1
Mol. weight [g/mol]:	170.59
CAS:	1642-81-5

Physical Properties

Property code	Value	Unit	Source
gf	-158.41	kJ/mol	Joback Method
hf	-263.94	kJ/mol	Joback Method
hfus	20.01	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.124		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	597.58	K	Joback Method
tc	809.04	K	Joback Method
tf	359.53	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.49	J/mol×K	597.58	Joback Method
cpg	266.08	J/mol×K	632.82	Joback Method
cpg	274.10	J/mol×K	668.07	Joback Method
cpg	281.58	J/mol×K	703.31	Joback Method
cpg	288.55	J/mol×K	738.55	Joback Method
cpg	295.02	J/mol×K	773.80	Joback Method
cpg	301.02	J/mol×K	809.04	Joback Method

dvisc	0.0036481	Pa×s	359.53	Joback Method
dvisc	0.0015134	Pa×s	399.21	Joback Method
dvisc	0.0007361	Pa×s	438.88	Joback Method
dvisc	0.0004034	Pa×s	478.55	Joback Method
dvisc	0.0002425	Pa×s	518.23	Joback Method
dvisc	0.0001567	Pa×s	557.90	Joback Method
dvisc	0.0001073	Pa×s	597.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1642815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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