

4-Chloro-o-anisic acid

Other names:	4-Chloro-o-anisic acid Benzoic acid, 4-chloro-2-methoxy-
Inchi:	InChI=1S/C8H7ClO3/c1-12-7-4-5(9)2-3-6(7)8(10)11/h2-4H,1H3,(H,10,11)
InchiKey:	UFEYMXHWIHFBRX-UHFFFAOYSA-N
Formula:	C8H7ClO3
SMILES:	COc1cc(Cl)ccc1C(=O)O
Mol. weight [g/mol]:	186.59

Physical Properties

Property code	Value	Unit	Source
hf	-476.79	kJ/mol	Cheméo Relay (1.0)
hfus	20.81	kJ/mol	Joback Method
hvap	92.07	kJ/mol	Cheméo Relay (1.0)
ie	8.89	eV	Cheméo Relay (1.0)
log10ws	-2.94		Cheméo Relay (1.0)
logp	2.047		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
tb	567.18	K	Cheméo Relay (1.0)
tf	409.24	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.43	J/mol×K	624.98	Joback Method
cpg	285.78	J/mol×K	659.99	Joback Method
cpg	293.65	J/mol×K	695.01	Joback Method
cpg	301.02	J/mol×K	730.02	Joback Method
cpg	307.91	J/mol×K	765.03	Joback Method
cpg	314.32	J/mol×K	800.05	Joback Method
cpg	320.26	J/mol×K	835.06	Joback Method
dvisc	0.0016343	Pa×s	394.28	Joback Method
dvisc	0.0007850	Pa×s	432.73	Joback Method
dvisc	0.0004250	Pa×s	471.18	Joback Method
dvisc	0.0002524	Pa×s	509.63	Joback Method

dvisc	0.0001613	Pa×s	548.08	Joback Method
dvisc	0.0001093	Pa×s	586.53	Joback Method
dvisc	0.0000777	Pa×s	624.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57479706&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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