

4-Chloro-ortho-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
CAS:	57479-70-6

Physical Properties

Property code	Value	Unit	Source
gf	-273.04	kJ/mol	Joback Method
hf	-407.63	kJ/mol	Joback Method
hfus	20.81	kJ/mol	Joback Method
hvap	67.22	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.047		Crippen Method
mvol	125.370	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	624.98	K	Joback Method
tc	835.06	K	Joback Method
tf	394.28	K	Joback Method
vc	0.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.43	J/molxK	624.98	Joback Method
cpg	314.32	J/molxK	800.05	Joback Method
cpg	307.91	J/molxK	765.03	Joback Method
cpg	301.02	J/molxK	730.02	Joback Method
cpg	293.65	J/molxK	695.01	Joback Method
cpg	285.78	J/molxK	659.99	Joback Method
cpg	320.26	J/molxK	835.06	Joback Method

dvisc	0.0000777	Paxs	624.98	Joback Method
dvisc	0.0001093	Paxs	586.53	Joback Method
dvisc	0.0001613	Paxs	548.08	Joback Method
dvisc	0.0002524	Paxs	509.63	Joback Method
dvisc	0.0004250	Paxs	471.18	Joback Method
dvisc	0.0007850	Paxs	432.73	Joback Method
dvisc	0.0016343	Paxs	394.28	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=C57479706&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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/65-919-0/4-Chloro-ortho-anisic-acid.pdf>

Generated by Cheméo on 2024-04-26 07:04:27.137012819 +0000 UTC m=+16404316.057590141.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.