2-Chloro-4,5-dimethylphenol

Other names:	Phenol, 2-chloro-4,5-dimethyl-
	Banol phenol
	2-Chloro-4,5-xylenol
	3,4-Dimethyl-6-chlorophenol
	3,4-Xylenol, 6-chloro-
	6-Chloro-3,4-xylenol
Inchi:	InChI=1S/C8H9ClO/c1-5-3-7(9)8(10)4-6(5)2/h3-4,10H,1-2H3
InchiKey:	PSOJLBXHRBFLLQ-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	Cc1cc(O)c(Cl)cc1C
Mol. weight [g/mol]:	156.61
CAS:	1124-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-56.92	kJ/mol	Joback Method
hf	-187.91	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.662		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	537.13	K	Joback Method
tc	770.68	K	Joback Method
tf	373.02	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.37	J/mol×K	537.13	Joback Method
cpg	292.19	J/mol×K	731.76	Joback Method
cpg	284.37	J/mol×K	692.83	Joback Method

cpg	276.06	J/mol×K	653.91	Joback Method
cpg	267.16	J/mol×K	614.98	Joback Method
cpg	257.62	J/mol×K	576.06	Joback Method
cpg	299.57	J/mol×K	770.68	Joback Method
dvisc	0.0000663	Pa×s	537.13	Joback Method
dvisc	0.0000957	Pa×s	509.78	Joback Method
dvisc	0.0001441	Pa×s	482.43	Joback Method
dvisc	0.0002279	Pa×s	455.07	Joback Method
dvisc	0.0003822	Pa×s	427.72	Joback Method
dvisc	0.0006878	Pa×s	400.37	Joback Method
dvisc	0.0013492	Pa×s	373.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124045&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

Latest version available from: