Phenol, 4-chloro-3,5-dimethyl-

Other names:	2-Chloro-5-hydroxy-1,3-dimethylbenzene
	2-Chloro-5-hydroxy-m-xylene
	2-Chloro-m-xylenol
	3,5-Dimethyl-4-chlorophenol
	3,5-Xylenol, 4-chloro-
	4-Chloro-1-hydroxy-3,5-dimethylbenzene
	4-Chloro-3,5-dimethylphenol
	4-Chloro-3,5-xylenol
	4-Chloro-m-xylenol
	Ayrtol
	Benzytol
	Camel
	Desson
	Dettol
	Dettol, liquid antiseptic
	Espadol
	Husept extra
	NSC 4971
	Nipacide PX
	Nipacide mx
	Ottasept
	Ottasept extra
	PCMX
	Para-chloro-meta-xylenol
	Parametaxylenol
	RBA 777
	Septiderm-hydrochloride
	Willenol V
	m-Xylenol, 4-chloro-
	p-Chloro-3,5-dimethylphenol
	p-Chloro-3,5-xylenol
	p-Chloro-m-xylenol
Inchi:	InChI=1S/C8H9ClO/c1-5-3-7(10)4-6(2)8(5)9/h3-4,10H,1-2H3
InchiKey:	OSDLLIBGSJNGJE-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	Cc1cc(O)cc(C)c1Cl
Mol. weight [g/mol]:	156.61

Physical Properties

Property code	Value	Unit	Source
hf	-192.47	kJ/mol	Cheméo Relay (1.0)
hfus	19.72	kJ/mol	Joback Method
hvap	71.19	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-2.80		Aqueous Solubility Prediction Method
logp	2.662		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
rinpol	1384.00		NIST Webbook
ripol	2561.00		NIST Webbook
tb	522.98	K	Cheméo Relay (1.0)
tc	763.89	K	Cheméo Relay (1.0)
tf	387.90	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.37	J/mol×K	537.13	Joback Method
cpg	299.57	J/mol×K	770.68	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
dvisc	0.0002279	Pa×s	455.08	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	0.0013492	Pa×s	373.02	Joback Method
dvisc	0.0003822	Pa×s	427.72	Joback Method
dvisc	0.0006878	Pa×s	400.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88040&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point