

4-Chloro-2,6-dimethylphenol

Other names:	4-Chloro-2,6-xylenol Phenol, 4-chloro-2,6-dimethyl- 2,6-Xylenol, 4-chloro- NSC 5785
Inchi:	InChI=1S/C8H9ClO/c1-5-3-7(9)4-6(2)8(5)10/h3-4,10H,1-2H3
InchiKey:	VWYKSJIPZHLNO-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	<chem>Cc1cc(Cl)cc(C)c1O</chem>
Mol. weight [g/mol]:	156.61
CAS:	1123-63-3

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.37	J/molxK	537.13	Joback Method
cpg	292.19	J/molxK	731.76	Joback Method
cpg	284.37	J/molxK	692.83	Joback Method
cpg	276.06	J/molxK	653.91	Joback Method
cpg	267.16	J/molxK	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	Paxs	537.13	Joback Method
dvisc	0.0000957	Paxs	509.78	Joback Method
dvisc	0.0001441	Paxs	482.43	Joback Method
dvisc	0.0002279	Paxs	455.07	Joback Method
dvisc	0.0003822	Paxs	427.72	Joback Method
dvisc	0.0006878	Paxs	400.37	Joback Method
dvisc	0.0013492	Paxs	373.02	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=C1123633&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
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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