

M-xylene, a,a'-diol 5-chloro-2-hydroxy-

Other names:	5-chloro-m-xylene-2, «alpha», «alpha»'-triol
Inchi:	InChI=1S/C8H9ClO3/c9-7-1-5(3-10)8(12)6(2-7)4-11/h1-2,10-12H,3-4H2
InchiKey:	OGMITUYZIACKHB-UHFFFAOYSA-N
Formula:	C8H9ClO3
SMILES:	OCc1cc(Cl)cc(CO)c1O
Mol. weight [g/mol]:	188.61
CAS:	17026-49-2

Physical Properties

Property code	Value	Unit	Source
gf	-330.56	kJ/mol	Joback Method
hf	-492.37	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	87.76	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.030		Crippen Method
mcvol	129.670	ml/mol	McGowan Method
pc	5183.17	kPa	Joback Method
tb	721.49	K	Joback Method
tc	923.43	K	Joback Method
tf	494.66	K	Joback Method
vc	0.428	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.50	J/molxK	721.49	Joback Method
cpg	332.34	J/molxK	755.15	Joback Method
cpg	338.86	J/molxK	788.80	Joback Method
cpg	345.11	J/molxK	822.46	Joback Method
cpg	351.12	J/molxK	856.12	Joback Method
cpg	356.96	J/molxK	889.78	Joback Method
cpg	362.68	J/molxK	923.43	Joback Method
dvisc	0.0001273	Paxs	494.66	Joback Method

dvisc	0.0000458	Paxs	532.46	Joback Method
dvisc	0.0000189	Paxs	570.27	Joback Method
dvisc	0.0000087	Paxs	608.08	Joback Method
dvisc	0.0000044	Paxs	645.88	Joback Method
dvisc	0.0000024	Paxs	683.68	Joback Method
dvisc	0.0000014	Paxs	721.49	Joback Method

Sources

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=C17026492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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