

1,4-Benzenedimethanol

Other names:	p-Xylene-«alpha», «alpha»'-diol «alpha», «alpha»'-p-Xylenediol p-(Hydroxymethyl)benzyl alcohol p-Benzenedimethanol p-Bis(hydroxymethyl)benzene p-Xylene glycol p-Xylylene glycol p-Xylylene-«alpha», «alpha»'-diol p-Xylylenediol Terephthalyl alcohol 1,4-Bis(hydroxymethyl)benzene 1,4-Dimethylolbenzene 1,4-Xylylene glycol «alpha», «alpha»'-Dihydroxy-p-xylene NSC 5097 p-phenylenedimethanol
Inchi:	InChI=1S/C8H10O2/c9-5-7-1-2-8(6-10)4-3-7/h1-4,9-10H,5-6H2
InchiKey:	BWVAOONFBYRHY-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	OCc1ccc(CO)cc1
Mol. weight [g/mol]:	138.16
CAS:	589-29-7

Physical Properties

Property code	Value	Unit	Source
chs	-4183.00 ± 2.00	kJ/mol	NIST Webbook
gf	-154.38	kJ/mol	Joback Method
hf	-287.85	kJ/mol	Joback Method
hfs	-394.00	kJ/mol	NIST Webbook
hfus	18.30	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	0.671		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
tb	598.46	K	Joback Method
tc	785.86	K	Joback Method

tf	340.50	K	Joback Method
vc	0.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.61	J/mol×K	598.46	Joback Method
cpg	306.14	J/mol×K	754.63	Joback Method
cpg	299.29	J/mol×K	723.39	Joback Method
cpg	292.04	J/mol×K	692.16	Joback Method
cpg	284.35	J/mol×K	660.93	Joback Method
cpg	276.22	J/mol×K	629.69	Joback Method
cpg	312.59	J/mol×K	785.86	Joback Method
dvisc	0.0000345	Paxs	598.46	Joback Method
dvisc	0.0000616	Paxs	555.47	Joback Method
dvisc	0.0001212	Paxs	512.47	Joback Method
dvisc	0.0002702	Paxs	469.48	Joback Method
dvisc	0.0007079	Paxs	426.49	Joback Method
dvisc	0.0023013	Paxs	383.49	Joback Method
dvisc	0.0100764	Paxs	340.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.70	K	0.10	NIST Webbook

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=C589297&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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