1,3-Benzenedimethanol

Other names:	m-xylene-«alpha»,«alpha»'-diol
Inchi:	InChI=1S/C8H10O2/c9-5-7-2-1-3-8(4-7)6-10/h1-4,9-10H,5-6H2
InchiKey:	YWMLORGQOFONNT-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	OCc1cccc(CO)c1
Mol. weight [g/mol]:	138.16
CAS:	626-18-6

Physical Properties

Property code	Value	Unit	Source
gf	-154.38	kJ/mol	Joback Method
hf	-287.85	kJ/mol	Joback Method
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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.61	J/mol×K	598.46	Joback Method
cpg	276.22	J/mol×K	629.69	Joback Method
cpg	284.35	J/mol×K	660.93	Joback Method
cpg	292.04	J/mol×K	692.16	Joback Method
cpg	299.29	J/mol×K	723.39	Joback Method
cpg	306.14	J/mol×K	754.63	Joback Method
cpg	312.59	J/mol×K	785.86	Joback Method
dvisc	0.0100764	Pa×s	340.50	Joback Method

dvisc	0.0023013	Pa×s	383.49	Joback Method
dvisc	0.0007079	Pa×s	426.49	Joback Method
dvisc	0.0002702	Pa×s	469.48	Joback Method
dvisc	0.0001212	Pa×s	512.47	Joback Method
dvisc	0.0000616	Pa×s	555.47	Joback Method
dvisc	0.0000345	Pa×s	598.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.70	K	1.70	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=C626186&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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