

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.61	J/molxK	598.46	Joback Method
cpg	306.14	J/molxK	754.63	Joback Method
cpg	299.29	J/molxK	723.39	Joback Method
cpg	292.04	J/molxK	692.16	Joback Method
cpg	284.35	J/molxK	660.93	Joback Method
cpg	276.22	J/molxK	629.69	Joback Method
cpg	312.59	J/molxK	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	429.70	K	1.70	NIST Webbook

Sources

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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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