1,4-Benzenedimethanol, «alpha»-methyl-

Other names: «alpha»-Methyl-1,4-benzenedimethanol
Inchi: InChI=1S/C9H12O2/c1-7(11)9-4-2-8(6-10)3-5-9/h2-5,7,10-11H,6H2,1H3
InchiKey: OZHROFCXIMHHRO-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CC(O)c1ccc(CO)cc1
Mol. weight [g/mol]: 152.19
CAS: 80463-22-5

Physical Properties

Property code	Value	Unit	Source
gf	-148.40	kJ/mol	Joback Method
hf	-313.77	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.232		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
rinpol	1422.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1411.00		NIST Webbook
tb	620.90	K	Joback Method
tc	809.67	K	Joback Method
tf	336.77	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.44	J/mol×K	620.90	Joback Method
cpg	324.06	J/mol×K	652.36	Joback Method
cpg	333.16	J/mol×K	683.82	Joback Method
cpg	341.75	J/mol×K	715.29	Joback Method
cpg	349.85	J/mol×K	746.75	Joback Method

cpg	357.48	J/mol×K	778.21	Joback Method
cpg	364.67	J/mol×K	809.67	Joback Method
dvisc	0.0136219	Pa×s	336.77	Joback Method
dvisc	0.0025131	Pa×s	384.12	Joback Method
dvisc	0.0006719	Pa×s	431.48	Joback Method
dvisc	0.0002332	Pa×s	478.84	Joback Method
dvisc	0.0000979	Pa×s	526.19	Joback Method
dvisc	0.0000474	Pa×s	573.54	Joback Method
dvisc	0.0000257	Pa×s	620.90	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80463225&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume