dl-2-Phenyl-1,2-propanediol

Other names:	1,2-Propanediol, 2-phenyl-
	1-Phenyl-1,2-propanediol
	1-Phenylpropane-1,2-diol
	DL-2-phenylpropane-1,2-diol
Inchi:	InChI=1S/C9H12O2/c1-9(11,7-10)8-5-3-2-4-6-8/h2-6,10-11H,7H2,1H3
InchiKey:	LNCZPZFNQQFXPT-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CC(O)(CO)c1ccccc1
Mol. weight [g/mol]:	152.19
CAS:	4217-66-7

Physical Properties

Property code	Value	Unit	Source
gf	-133.49	kJ/mol	Joback Method
hf	-305.77	kJ/mol	Joback Method
hfus	13.87	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.886		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
ripol	2339.00		NIST Webbook
ripol	2343.00		NIST Webbook
tb	613.13	K	Joback Method
tc	807.24	K	Joback Method
tf	341.67	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.72	J/mol×K	613.13	Joback Method
cpg	362.40	J/mol×K	774.89	Joback Method
cpg	354.82	J/mol×K	742.53	Joback Method

cpg	346.71	J/mol×K	710.18	Joback Method
cpg	338.01	J/mol×K	677.83	Joback Method
cpg	328.70	J/mol×K	645.48	Joback Method
cpg	369.49	J/mol×K	807.24	Joback Method
dvisc	0.0000261	Pa×s	613.13	Joback Method
dvisc	0.0000491	Pa×s	567.89	Joback Method
dvisc	0.0001031	Pa×s	522.64	Joback Method
dvisc	0.0002494	Pa×s	477.40	Joback Method
dvisc	0.0007257	Pa×s	432.16	Joback Method
dvisc	0.0027111	Pa×s	386.91	Joback Method
dvisc	0.0143595	Pa×s	341.67	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4217667&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume