

1,2-PROPANEDIOL, 2-PHENYL-

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

Physical Properties

Property code	Value	Unit	Source
af	0.7436		Cheméo Relay (1.0)
hf	-314.54	kJ/mol	Cheméo Relay (1.0)
hfus	13.87	kJ/mol	Joback Method
hvap	89.99	kJ/mol	Cheméo Relay (1.0)
ie	8.93	eV	Cheméo Relay (1.0)
log10ws	-0.88		Cheméo Relay (1.0)
logp	0.886		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
ripol	2343.00		NIST Webbook
ripol	2339.00		NIST Webbook
tb	540.98	K	Cheméo Relay (1.0)
tc	775.60	K	Cheméo Relay (1.0)
tf	338.11	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.72	J/mol×K	613.13	Joback Method
cpg	369.49	J/mol×K	807.24	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
dvisc	0.0002494	Pa×s	477.40	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	0.0143595	Pa×s	341.67	Joback Method
dvisc	0.0007257	Pa×s	432.16	Joback Method
dvisc	0.0027111	Pa×s	386.91	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4217667&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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