

1-phenylpropane-1,2-diol

Inchi:	InChI=1S/C9H12O2/c1-7(10)9(11)8-5-3-2-4-6-8/h2-7,9-11H,1H3
InchiKey:	MZQZXSHFWDHNOW-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CC(O)C(O)c1ccccc1
Mol. weight [g/mol]:	152.19
CAS:	1855-09-0

Physical Properties

Property code	Value	Unit	Source
gf	-141.21	kJ/mol	Joback Method
hf	-307.58	kJ/mol	Joback Method
hfus	14.24	kJ/mol	Joback Method
hvap	70.49	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.101		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
rinpol	1326.60		NIST Webbook
tb	615.48	K	Joback Method
tc	806.73	K	Joback Method
tf	309.25	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.07	J/molxK	615.48	Joback Method
cpg	326.11	J/molxK	647.35	Joback Method
cpg	335.54	J/molxK	679.23	Joback Method
cpg	344.41	J/molxK	711.10	Joback Method
cpg	352.74	J/molxK	742.98	Joback Method
cpg	360.56	J/molxK	774.85	Joback Method
cpg	367.90	J/molxK	806.73	Joback Method
dvisc	0.0489968	Paxs	309.25	Joback Method

dvisc	0.0056746	Paxs	360.29	Joback Method
dvisc	0.0011221	Paxs	411.33	Joback Method
dvisc	0.0003174	Paxs	462.37	Joback Method
dvisc	0.0001154	Paxs	513.40	Joback Method
dvisc	0.0000504	Paxs	564.44	Joback Method
dvisc	0.0000252	Paxs	615.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1855090&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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