dl-Erythro-1-phenyl-1,2-propanediol

Other names: erythro-1-Phenylpropane-1,2-diol
1-phenyl-1,2-propanediol
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: 1075-04-3

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
ripol	2361.00		NIST Webbook
ripol	2361.00		NIST Webbook
ripol	2365.00		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/mol×K	615.48	Joback Method
cpg	326.11	J/mol×K	647.35	Joback Method
cpg	335.54	J/mol×K	679.23	Joback Method
cpg	344.41	J/mol×K	711.10	Joback Method

cpg	352.74	J/mol×K	742.98	Joback Method
cpg	360.56	J/mol×K	774.85	Joback Method
cpg	367.90	J/mol×K	806.73	Joback Method
dvisc	0.0489968	Pa×s	309.25	Joback Method
dvisc	0.0056746	Pa×s	360.29	Joback Method
dvisc	0.0011221	Pa×s	411.33	Joback Method
dvisc	0.0003174	Pa×s	462.37	Joback Method
dvisc	0.0001154	Pa×s	513.40	Joback Method
dvisc	0.0000504	Pa×s	564.44	Joback Method
dvisc	0.0000252	Pa×s	615.48	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1075043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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