1-phenylbutane-2,3-diol

Other names: 1-Phenylbutan-2,3-diol
Inchi: InChI=1S/C10H14O2/c1-8(11)10(12)7-9-5-3-2-4-6-9/h2-6,8,10-12H,7H2,1H3
InchiKey: WHYBHJWYBIXOPS-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC(O)C(O)Cc1ccccc1
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-132.79	kJ/mol	Joback Method
hf	-328.22	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	72.71	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	0.971		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
rinpol	1419.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	638.36	K	Joback Method
tc	827.59	K	Joback Method
tf	320.52	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.00	J/mol×K	638.36	Joback Method
cpg	374.74	J/mol×K	669.90	Joback Method
cpg	384.85	J/mol×K	701.44	Joback Method
cpg	394.37	J/mol×K	732.97	Joback Method
cpg	403.32	J/mol×K	764.51	Joback Method
cpg	411.74	J/mol×K	796.05	Joback Method

cpg	419.64	J/mol×K	827.59	Joback Method
dvisc	0.0344533	Pa×s	320.52	Joback Method
dvisc	0.0041183	Pa×s	373.49	Joback Method
dvisc	0.0008344	Pa×s	426.47	Joback Method
dvisc	0.0002406	Pa×s	479.44	Joback Method
dvisc	0.0000888	Pa×s	532.41	Joback Method
dvisc	0.0000393	Pa×s	585.39	Joback Method
dvisc	0.0000199	Pa×s	638.36	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R225255&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

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