1-Phenylcyclopentane-cis-1,2-diol

Inchi: InChI=1S/C11H14O2/c12-10-7-4-8-11(10,13)9-5-2-1-3-6-9/h1-3,5-6,10,12-13H,4,7-8H2
InchiKey: CWTWKJLRHPCTRR-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: OC1CCCC1(O)c1ccccc1
Mol. weight [g/mol]: 178.23
CAS: 81155-86-4

Physical Properties

Property code	Value	Unit	Source
chs	-5910.30 ± 4.20	kJ/mol	NIST Webbook
chs	-5916.60	kJ/mol	NIST Webbook
gf	-96.14	kJ/mol	Joback Method
hf	-282.92	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	74.51	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.419		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	672.97	K	Joback Method
tc	882.35	K	Joback Method
tf	392.35	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.53	J/mol×K	672.97	Joback Method
cpg	412.01	J/mol×K	707.87	Joback Method
cpg	423.85	J/mol×K	742.76	Joback Method
cpg	435.17	J/mol×K	777.66	Joback Method
cpg	446.09	J/mol×K	812.56	Joback Method
cpg	456.73	J/mol×K	847.45	Joback Method
cpg	467.20	J/mol×K	882.35	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=C81155864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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