1,2-Cyclohexanediol, 1-phenyl-, trans-

Other names: 1-Phenyl-trans-1,2-cyclohexanediol
Inchi: InChI=1S/C12H16O2/c13-11-8-4-5-9-12(11,14)10-6-2-1-3-7-10/h1-3,6-7,11,13-14H,4-5,8
InchiKey: QHNHEYDAIICUDL-NWDGAFQWSA-N
Formula: C12H16O2
SMILES: OC1CCCCC1(O)c1ccccc1
Mol. weight [g/mol]: 192.25
CAS: 27167-34-6

Physical Properties

Property code	Value	Unit	Source
chs	-6536.70 ± 0.80	kJ/mol	NIST Webbook
chs	-6543.80	kJ/mol	NIST Webbook
gf	-99.82	kJ/mol	Joback Method
hf	-309.72	kJ/mol	Joback Method
hfus	15.66	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.809		Crippen Method
mcvol	157.060	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	700.12	K	Joback Method
tc	912.50	K	Joback Method
tf	400.10	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.96	J/mol×K	700.12	Joback Method
cpg	466.74	J/mol×K	735.52	Joback Method
cpg	479.83	J/mol×K	770.91	Joback Method
cpg	492.35	J/mol×K	806.31	Joback Method
cpg	504.44	J/mol×K	841.71	Joback Method
cpg	516.21	J/mol×K	877.10	Joback Method

cpg	527.78	J/mol×K	912.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27167346&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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