1-Phenylcyclohexanol

Other names: Cyclohexanol, 1-phenyl-
1-Phenyl-1-cyclohexanol
1-Phenylcyclohexanol-1
Benzene, cyclohex-1-yl-1-ol-
Inchi: InChI=1S/C12H16O/c13-12(9-5-2-6-10-12)11-7-3-1-4-8-11/h1,3-4,7-8,13H,2,5-6,9-10H2
InchiKey: DTTDXHDYTWQDCS-UHFFFAOYSA-N
Formula: C12H16O
SMILES: OC1(c2ccccc2)CCCCC1
Mol. weight [g/mol]: 176.25
CAS: 1589-60-2

Physical Properties

Property code	Value	Unit	Source
gf	44.71	kJ/mol	Joback Method
hf	-137.15	kJ/mol	Joback Method
hfus	10.50	kJ/mol	Joback Method
hvap	60.54	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
log10ws	-3.28		Crippen Method
logp	2.838		Crippen Method
mcvol	151.190	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	612.61	K	Joback Method
tc	842.12	K	Joback Method
tf	333.00 ± 4.00	K	NIST Webbook
tf	333.00 ± 3.00	K	NIST Webbook
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.22	J/mol×K	612.61	Joback Method
cpg	410.80	J/mol×K	650.86	Joback Method
cpg	426.27	J/mol×K	689.11	Joback Method

cpg	440.80	J/mol×K	727.36	Joback Method
cpg	454.54	J/mol×K	765.61	Joback Method
cpg	467.65	J/mol×K	803.87	Joback Method
cpg	480.29	J/mol×K	842.12	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=C1589602&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
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
ie:	Ionization energy
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