1-Phenylcyclopentanol-1

Other names: Cyclopentanol, 1-phenyl-
1-Phenylcyclopentanol
Benzene, cyclopent-1-yl-1-ol-
Inchi: InChI=1S/C11H14O/c12-11(8-4-5-9-11)10-6-2-1-3-7-10/h1-3,6-7,12H,4-5,8-9H2
InchiKey: ITHZGJVAQFFNCZ-UHFFFAOYSA-N
Formula: C11H14O
SMILES: OC1(c2ccccc2)CCCC1
Mol. weight [g/mol]: 162.23
CAS: 10487-96-4

Physical Properties

Property code	Value	Unit	Source
gf	48.39	kJ/mol	Joback Method
hf	-110.35	kJ/mol	Joback Method
hfus	10.01	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
log10ws	-2.86		Crippen Method
logp	2.448		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	585.46	K	Joback Method
tc	811.58	K	Joback Method
tf	335.77	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.09	J/mol×K	585.46	Joback Method
cpg	359.18	J/mol×K	623.15	Joback Method
cpg	373.22	J/mol×K	660.83	Joback Method
cpg	386.34	J/mol×K	698.52	Joback Method
cpg	398.71	J/mol×K	736.20	Joback Method

cpg	410.49	J/mol×K	773.89	Joback Method
cpg	421.84	J/mol×K	811.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.70	K	2.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10487964&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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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