1-Methyl-1-phenylcyclobutane

Other names: Benzene, (1-methylcyclobutyl)-
Inchi: InChI=1S/C11H14/c1-11(8-5-9-11)10-6-3-2-4-7-10/h2-4,6-7H,5,8-9H2,1H3
InchiKey: GRDSPXXZEBFXHZ-UHFFFAOYSA-N
Formula: C11H14
SMILES: CC1(c2ccccc2)CCC1
Mol. weight [g/mol]: 146.23
CAS: 7306-05-0

Physical Properties

Property code	Value	Unit	Source
gf	197.31	kJ/mol	Joback Method
hf	48.04	kJ/mol	Joback Method
hfus	8.02	kJ/mol	Joback Method
hvap	41.29	kJ/mol	Joback Method
ie	8.10	eV	NIST Webbook
log10ws	-3.10		Crippen Method
logp	3.128		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	481.80 ± 0.50	K	NIST Webbook
tc	726.35	K	Joback Method
tf	278.47	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.92	J/mol×K	489.01	Joback Method
cpg	304.36	J/mol×K	528.57	Joback Method
cpg	321.24	J/mol×K	568.12	Joback Method
cpg	336.74	J/mol×K	607.68	Joback Method
cpg	351.07	J/mol×K	647.24	Joback Method
cpg	364.40	J/mol×K	686.80	Joback Method
cpg	376.92	J/mol×K	726.35	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=C7306050&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