Benzene, 2-cyclohexen-1-yl-

Other names:	3-Phenyl-1-cyclohexene
	3-Phenylcyclohexene
Inchi:	InChI=1S/C12H14/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1,3-5,7-9,12H,2,6,10H2
InchiKey:	MUSXBUOOSTWNCY-UHFFFAOYSA-N
Formula:	C12H14
SMILES:	C1=CC(c2ccccc2)CCC1
Mol. weight [g/mol]:	158.24
CAS:	15232-96-9

Physical Properties

Property code	Value	Unit	Source
gf	216.98	kJ/mol	Joback Method
hf	57.62	kJ/mol	Joback Method
hfus	13.93	kJ/mol	Joback Method
hvap	45.30	kJ/mol	Joback Method
ie	7.96 ± 0.02	eV	NIST Webbook
log10ws	-3.66		Crippen Method
logp	3.510		Crippen Method
mcvol	141.020	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	519.35	K	Joback Method
tc	762.70	K	Joback Method
tf	259.56	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.09	J/mol×K	519.35	Joback Method
cpg	335.13	J/mol×K	559.91	Joback Method
cpg	353.72	J/mol×K	600.47	Joback Method
cpg	370.92	J/mol×K	641.02	Joback Method
cpg	386.81	J/mol×K	681.58	Joback Method
cpg	401.46	J/mol×K	722.14	Joback Method

cpg	414.92	J/mol×K	762.70	Joback Method
dvisc	0.0041071	Pa×s	259.56	Joback Method
dvisc	0.0017955	Pa×s	302.86	Joback Method
dvisc	0.0009654	Pa×s	346.16	Joback Method
dvisc	0.0005959	Pa×s	389.46	Joback Method
dvisc	0.0004051	Pa×s	432.75	Joback Method
dvisc	0.0002954	Pa×s	476.05	Joback Method
dvisc	0.0002271	Pa×s	519.35	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15232969&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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