Benzene, 3-cyclohexen-1-yl-

Other names: 4-Phenylcyclohexene
Inchi: InChI=1S/C12H14/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-5,7-8,12H,6,9-10H2
InchiKey: XWCWNUSFQVJNDI-UHFFFAOYSA-N
Formula: C12H14
SMILES: C1=CCC(c2ccccc2)CC1
Mol. weight [g/mol]: 158.24
CAS: 4994-16-5

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	8.57 ± 0.01	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
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1800.00		NIST Webbook
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

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=C4994165&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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume