

Cyclohexene,1-cyclohexyl-

Inchi:	InChI=1S/C12H20/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h7,12H,1-6,8-10H2
InchiKey:	RFFCUDDJJDOFLS-UHFFFAOYSA-N
Formula:	C12H20
SMILES:	C1=C(C2CCCCC2)CCCC1
Mol. weight [g/mol]:	164.29
CAS:	3282-54-0

Physical Properties

Property code	Value	Unit	Source
gf	127.10	kJ/mol	Joback Method
hf	-115.72	kJ/mol	Joback Method
hfus	10.27	kJ/mol	Joback Method
hvap	44.43	kJ/mol	Joback Method
ie	8.30 ± 0.01	eV	NIST Webbook
log10ws	-4.25		Crippen Method
logp	4.067		Crippen Method
mcvol	153.920	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	521.87	K	Joback Method
tc	757.67	K	Joback Method
tf	257.28	K	Joback Method
vc	0.560	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.53	J/mol×K	521.87	Joback Method
cpg	473.13	J/mol×K	718.37	Joback Method
cpg	455.07	J/mol×K	679.07	Joback Method
cpg	435.63	J/mol×K	639.77	Joback Method
cpg	414.77	J/mol×K	600.47	Joback Method
cpg	392.42	J/mol×K	561.17	Joback Method
cpg	489.87	J/mol×K	757.67	Joback Method
dvisc	0.0002266	Paxs	521.87	Joback Method

dvisc	0.0003110	Paxs	477.77	Joback Method
dvisc	0.0004552	Paxs	433.67	Joback Method
dvisc	0.0007262	Paxs	389.57	Joback Method
dvisc	0.0013053	Paxs	345.48	Joback Method
dvisc	0.0027853	Paxs	301.38	Joback Method
dvisc	0.0077070	Paxs	257.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3282540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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