Cyclohexene,3-cyclohexyl-

Inchi: InChI=1S/C12H20/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h3,7,11-12H,1-2,4-6,8-10H2
InchiKey: KWMKLXOPDTWVIT-UHFFFAOYSA-N
Formula: C12H20
SMILES: C1=CC(C2CCCCC2)CCC1
Mol. weight [g/mol]: 164.29
CAS: 1808-09-9

Physical Properties

Property code	Value	Unit	Source
gf	129.02	kJ/mol	Joback Method
hf	-124.59	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	43.46	kJ/mol	Joback Method
ie	8.68 ± 0.01	eV	NIST Webbook
log10ws	-4.01		Crippen Method
logp	3.923		Crippen Method
mcvol	153.920	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	512.22	K	Joback Method
tc	746.70	K	Joback Method
tf	240.52	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.46	J/mol×K	512.22	Joback Method
cpg	476.31	J/mol×K	707.62	Joback Method
cpg	457.51	J/mol×K	668.54	Joback Method
cpg	437.28	J/mol×K	629.46	Joback Method
cpg	415.56	J/mol×K	590.38	Joback Method
cpg	392.31	J/mol×K	551.30	Joback Method
cpg	493.75	J/mol×K	746.70	Joback Method
dvisc	0.0002545	Pa×s	512.22	Joback Method

dvisc	0.0003441	Pa×s	466.94	Joback Method
dvisc	0.0004964	Pa×s	421.65	Joback Method
dvisc	0.0007822	Pa×s	376.37	Joback Method
dvisc	0.0013955	Pa×s	331.09	Joback Method
dvisc	0.0029911	Pa×s	285.80	Joback Method
dvisc	0.0085432	Pa×s	240.52	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=C1808099&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