Cyclohexyl radical

Inchi: InChI=1S/C6H11/c1-2-4-6-5-3-1/h1H,2-6H2
InchiKey: YUDRVAHLXDBKSR-UHFFFAOYSA-N
Formula: C6H11
SMILES: [CH]1CCCCC1
Mol. weight [g/mol]: 83.15
CAS: 3170-58-9

Physical Properties

Property code	Value	Unit	Source
ea	-0.24 ± 0.11	eV	NIST Webbook
gf	76.47	kJ/mol	Joback Method
hf	-57.04	kJ/mol	Joback Method
hfus	4.81	kJ/mol	Joback Method
hvap	29.23	kJ/mol	Joback Method
ie	7.66 ± 0.05	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	2.155		Crippen Method
mcvol	82.390	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	355.53	K	Joback Method
tc	555.38	K	Joback Method
tf	181.13	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.80	J/mol×K	355.53	Joback Method
cpg	192.86	J/mol×K	522.07	Joback Method
cpg	181.59	J/mol×K	488.76	Joback Method
cpg	169.59	J/mol×K	455.46	Joback Method
cpg	156.82	J/mol×K	422.15	Joback Method
cpg	143.23	J/mol×K	388.84	Joback Method
cpg	203.44	J/mol×K	555.38	Joback Method

dvisc	0.0003402	Pa×s	355.53	Joback Method
dvisc	0.0003900	Pa×s	326.46	Joback Method
dvisc	0.0004592	Pa×s	297.40	Joback Method
dvisc	0.0005602	Pa×s	268.33	Joback Method
dvisc	0.0007172	Pa×s	239.26	Joback Method
dvisc	0.0009830	Pa×s	210.20	Joback Method
dvisc	0.0014908	Pa×s	181.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3170589&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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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