Cyclohexene,1-propyl-

Other names: 1-Propyl-1-cyclohexene
1-Propylcyclohexene-1
Inchi: InChI=1S/C9H16/c1-2-6-9-7-4-3-5-8-9/h7H,2-6,8H2,1H3
InchiKey: WCPWJMLXSZIWOP-UHFFFAOYSA-N
Formula: C9H16
SMILES: CCCC1=CCCCC1
Mol. weight [g/mol]: 124.22
CAS: 2539-75-5

Physical Properties

Property code	Value	Unit	Source
gf	77.39	kJ/mol	Joback Method
hf	-108.12	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	37.32	kJ/mol	Joback Method
ie	8.43 ± 0.01	eV	NIST Webbook
log10ws	-3.34		Crippen Method
logp	3.287		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	954.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	949.60		NIST Webbook
rinpol	944.50		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	979.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1076.00		NIST Webbook
ripol	1090.80		NIST Webbook
ripol	1094.00		NIST Webbook

ripol	1075.80		NIST Webbook
ripol	1081.40		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1099.60		NIST Webbook
ripol	1079.30		NIST Webbook
ripol	1090.20		NIST Webbook
ripol	1099.60		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1090.20		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1079.00		NIST Webbook
ripol	1081.00		NIST Webbook
ripol	1086.40		NIST Webbook
tb	427.20 ± 4.00	K	NIST Webbook
tb	429.40 ± 5.00	K	NIST Webbook
tc	636.54	K	Joback Method
tf	216.09	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.01	J/mol×K	433.68	Joback Method
cpg	317.78	J/mol×K	602.73	Joback Method
cpg	304.38	J/mol×K	568.92	Joback Method
cpg	290.23	J/mol×K	535.11	Joback Method
cpg	275.31	J/mol×K	501.30	Joback Method
cpg	259.57	J/mol×K	467.49	Joback Method
cpg	330.45	J/mol×K	636.54	Joback Method
dvisc	0.0002509	Pa×s	433.68	Joback Method
dvisc	0.0003357	Pa×s	397.41	Joback Method
dvisc	0.0004761	Pa×s	361.15	Joback Method
dvisc	0.0007299	Pa×s	324.88	Joback Method
dvisc	0.0012461	Pa×s	288.62	Joback Method
dvisc	0.0024807	Pa×s	252.35	Joback Method
dvisc	0.0062223	Pa×s	216.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2539755&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol647.mol

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