1-Isopropylcyclohex-1-ene

Other names:	Cyclohexene, 1-(1-methylethyl)
	1-Isopropylcyclohexene-1
	1-isopropylcyclohexene
Inchi:	InChI=1S/C9H16/c1-8(2)9-6-4-3-5-7-9/h6,8H,3-5,7H2,1-2H3
InchiKey:	ZYMCVIZKLGUPBG-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CC(C)C1=CCCCC1
Mol. weight [g/mol]:	124.22
CAS:	4292-04-0

Physical Properties

Property code	Value	Unit	Source
gf	74.95	kJ/mol	Joback Method
hf	-113.40	kJ/mol	Joback Method
hfus	7.14	kJ/mol	Joback Method
hvap	36.93	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.143		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	922.20		NIST Webbook
rinpol	928.80		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	922.80		NIST Webbook
rinpol	919.40		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	972.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1082.30		NIST Webbook
ripol	1058.10		NIST Webbook
ripol	1069.80		NIST Webbook
ripol	1055.00		NIST Webbook
ripol	1073.00		NIST Webbook
ripol	1064.00		NIST Webbook
ripol	1038.00		NIST Webbook

ripol	1045.00		NIST Webbook
tb	426.30 ± 4.00	K	NIST Webbook
tb	429.00 ± 5.00	K	NIST Webbook
tc	641.00	K	Joback Method
tf	201.09	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.03	J/mol×K	433.24	Joback Method
cpg	319.80	J/mol×K	606.37	Joback Method
cpg	306.09	J/mol×K	571.75	Joback Method
cpg	291.59	J/mol×K	537.12	Joback Method
cpg	276.27	J/mol×K	502.49	Joback Method
cpg	260.09	J/mol×K	467.87	Joback Method
cpg	332.73	J/mol×K	641.00	Joback Method
dvisc	0.0002403	Pa×s	433.24	Joback Method
dvisc	0.0003314	Pa×s	394.55	Joback Method
dvisc	0.0004902	Pa×s	355.86	Joback Method
dvisc	0.0007978	Pa×s	317.17	Joback Method
dvisc	0.0014865	Pa×s	278.47	Joback Method
dvisc	0.0033858	Pa×s	239.78	Joback Method
dvisc	0.0105863	Pa×s	201.09	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4292040&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
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
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