

Cyclohexene,3-propyl-

Other names:	3-Propylcyclohexene-1 3-Propyl-1-cyclohexene
Inchi:	InChI=1S/C9H16/c1-2-6-9-7-4-3-5-8-9/h4,7,9H,2-3,5-6,8H2,1H3
InchiKey:	XWIMYKYUBWUJOH-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CCCC1C=CCCC1
Mol. weight [g/mol]:	124.22
CAS:	3983-06-0

Physical Properties

Property code	Value	Unit	Source
gf	79.31	kJ/mol	Joback Method
hf	-116.99	kJ/mol	Joback Method
hfus	12.12	kJ/mol	Joback Method
hvap	36.35	kJ/mol	Joback Method
ie	8.80 ± 0.01	eV	NIST Webbook
log10ws	-3.10		Crippen Method
logp	3.143		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	944.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	938.50		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	944.40		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	948.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1097.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1097.00		NIST Webbook
ripol	1076.40		NIST Webbook
ripol	1070.80		NIST Webbook
ripol	1091.80		NIST Webbook
ripol	1087.20		NIST Webbook

ripol	1085.40		NIST Webbook
ripol	1082.20		NIST Webbook
ripol	1076.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1087.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1097.00		NIST Webbook
ripol	1085.40		NIST Webbook
ripol	1097.00		NIST Webbook
ripol	1082.00		NIST Webbook
tb	424.03	K	Joback Method
tc	625.02	K	Joback Method
tf	199.33	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.41	J/mol×K	424.03	Joback Method
cpg	319.82	J/mol×K	591.52	Joback Method
cpg	305.76	J/mol×K	558.03	Joback Method
cpg	290.92	J/mol×K	524.53	Joback Method
cpg	275.26	J/mol×K	491.03	Joback Method
cpg	258.77	J/mol×K	457.53	Joback Method
cpg	333.12	J/mol×K	625.02	Joback Method
dvisc	0.0002623	Pa×s	424.03	Joback Method
dvisc	0.0003440	Pa×s	386.58	Joback Method
dvisc	0.0004781	Pa×s	349.13	Joback Method
dvisc	0.0007191	Pa×s	311.68	Joback Method
dvisc	0.0012094	Pa×s	274.23	Joback Method
dvisc	0.0023974	Pa×s	236.78	Joback Method
dvisc	0.0061457	Pa×s	199.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3983060&Units=SI

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

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