

Cyclohexene, 3-(2-methylpropyl)-

Other names:	Cyclohexene, 3-isobutyl- 3-Isobutyl-1-cyclohexene 3-Isobutylcyclohexene-1
Inchi:	InChI=1S/C10H18/c1-9(2)8-10-6-4-3-5-7-10/h4,6,9-10H,3,5,7-8H2,1-2H3
InchiKey:	NVLNRIBMCIJLQD-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	CC(C)CC1C=CCCC1
Mol. weight [g/mol]:	138.25
CAS:	4104-56-7

Physical Properties

Property code	Value	Unit	Source
gf	85.29	kJ/mol	Joback Method
hf	-142.91	kJ/mol	Joback Method
hfus	11.19	kJ/mol	Joback Method
hvap	38.19	kJ/mol	Joback Method
ie	8.77 ± 0.02	eV	NIST Webbook
log10ws	-3.27		Crippen Method
logp	3.389		Crippen Method
mcvol	136.600	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1025.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	998.20		NIST Webbook
rinpol	992.50		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	998.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1117.90		NIST Webbook
ripol	1105.80		NIST Webbook
ripol	1127.70		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1156.00		NIST Webbook
tb	446.47	K	Joback Method

tc	649.96	K	Joback Method
tf	195.60	K	Joback Method
vc	0.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.13	J/mol×K	446.47	Joback Method
cpg	303.97	J/mol×K	480.39	Joback Method
cpg	321.85	J/mol×K	514.30	Joback Method
cpg	338.80	J/mol×K	548.22	Joback Method
cpg	354.85	J/mol×K	582.13	Joback Method
cpg	370.02	J/mol×K	616.05	Joback Method
cpg	384.34	J/mol×K	649.96	Joback Method
dvisc	0.0107831	Pa×s	195.60	Joback Method
dvisc	0.0032902	Pa×s	237.41	Joback Method
dvisc	0.0014325	Pa×s	279.22	Joback Method
dvisc	0.0007745	Pa×s	321.04	Joback Method
dvisc	0.0004825	Pa×s	362.85	Joback Method
dvisc	0.0003315	Pa×s	404.66	Joback Method
dvisc	0.0002443	Pa×s	446.47	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=C4104567&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
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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