

Cyclohexane, 1-isopropyl-1-methyl-

Inchi:	InChI=1S/C10H20/c1-9(2)10(3)7-5-4-6-8-10/h9H,4-8H2,1-3H3
InchiKey:	XWPBAJRHMYWMKT-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CC(C)C1(C)CCCCC1
Mol. weight [g/mol]:	140.27
CAS:	16580-26-0

Physical Properties

Property code	Value	Unit	Source
gf	49.84	kJ/mol	Joback Method
hf	-185.45	kJ/mol	Joback Method
hfus	3.67	kJ/mol	Joback Method
hvap	36.74	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.613		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
tb	450.70 ± 1.00	K	NIST Webbook
tc	657.97	K	Joback Method
tf	218.74	K	Joback Method
vc	0.520	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.80	J/mol×K	447.55	Joback Method
cpg	321.33	J/mol×K	482.62	Joback Method
cpg	340.55	J/mol×K	517.69	Joback Method
cpg	358.55	J/mol×K	552.76	Joback Method
cpg	375.45	J/mol×K	587.83	Joback Method
cpg	391.35	J/mol×K	622.90	Joback Method
cpg	406.36	J/mol×K	657.97	Joback Method

Sources

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=C16580260&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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