

Cyclohexane, 1-(cyclohexylmethyl)-4-(1-methylethyl)-

Other names: Cyclohexane, 1-(cyclohexylmethyl)-4-(1-methylethyl)-
Methane, cyclohexyl(4-isopropylcyclohexyl)-

Inchi: InChI=1S/C16H30/c1-13(2)16-10-8-15(9-11-16)12-14-6-4-3-5-7-14/h13-16H,3-12H2,1-2H3

InchiKey: LHWJKUKEUOFSME-UHFFFAOYSA-N

Formula: C16H30

SMILES: CC(C)C1CCC(CC2CCCCC2)CC1

Mol. weight [g/mol]: 222.42

Physical Properties

Property code	Value	Unit	Source
af	0.3956		Cheméo Relay (1.0)
chs	-10180.00	kJ/mol	NIST Webbook
chs	-10200.00	kJ/mol	NIST Webbook
gf	122.59	kJ/mol	Joback Method
hf	-315.62	kJ/mol	Cheméo Relay (1.0)
hfus	18.41	kJ/mol	Joback Method
hvap	70.89	kJ/mol	Cheméo Relay (1.0)
ie	9.25	eV	Cheméo Relay (1.0)
log10ws	-6.80		Cheméo Relay (1.0)
logp	5.419		Crippen Method
mcvol	214.580	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
tb	573.11	K	Cheméo Relay (1.0)
tc	772.79	K	Cheméo Relay (1.0)
tf	259.51	K	Cheméo Relay (1.0)
vc	0.775	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.79	J/mol×K	599.47	Joback Method
cpg	629.69	J/mol×K	636.18	Joback Method
cpg	655.89	J/mol×K	672.89	Joback Method
cpg	680.43	J/mol×K	709.60	Joback Method

cpg	703.37	J/mol×K	746.30	Joback Method
cpg	724.75	J/mol×K	783.01	Joback Method
cpg	744.63	J/mol×K	819.72	Joback Method
dvisc	0.0091891	Pa×s	265.60	Joback Method
dvisc	0.0027396	Pa×s	321.25	Joback Method
dvisc	0.0011676	Pa×s	376.89	Joback Method
dvisc	0.0006197	Pa×s	432.54	Joback Method
dvisc	0.0003800	Pa×s	488.18	Joback Method
dvisc	0.0002576	Pa×s	543.83	Joback Method
dvisc	0.0001876	Pa×s	599.47	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54965616&Units=SI

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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