

Cyclohexane, 1-methylhexyl

Inchi:	InChI=1S/C13H26/c1-3-4-6-9-12(2)13-10-7-5-8-11-13/h12-13H,3-11H2,1-2H3
InchiKey:	AROVDVSKSDBION-UHFFFAOYSA-N
Formula:	C13H26
SMILES:	CCCCC(C)C1CCCCC1
Mol. weight [g/mol]:	182.35

Physical Properties

Property code	Value	Unit	Source
gf	80.59	kJ/mol	Joback Method
hf	-262.61	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	44.57	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.783		Crippen Method
mcvol	183.170	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1362.00		NIST Webbook
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tb	515.95	K	Joback Method
tc	709.95	K	Joback Method
tf	228.65	K	Joback Method
vc	0.691	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.63	J/molxK	515.95	Joback Method
cpg	467.60	J/molxK	548.28	Joback Method
cpg	488.49	J/molxK	580.62	Joback Method
cpg	508.34	J/molxK	612.95	Joback Method
cpg	527.16	J/molxK	645.28	Joback Method
cpg	545.00	J/molxK	677.61	Joback Method
cpg	561.88	J/molxK	709.95	Joback Method
dvisc	0.0127535	Paxs	228.65	Joback Method

dvisc	0.0035288	Paxs	276.53	Joback Method
dvisc	0.0014268	Paxs	324.42	Joback Method
dvisc	0.0007282	Paxs	372.30	Joback Method
dvisc	0.0004332	Paxs	420.18	Joback Method
dvisc	0.0002866	Paxs	468.07	Joback Method
dvisc	0.0002047	Paxs	515.95	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=R133265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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