

1-Methyl-2-pentyl cyclohexene

Inchi:	InChI=1S/C12H22/c1-3-4-5-9-12-10-7-6-8-11(12)2/h3-10H2,1-2H3
InchiKey:	FLJTYZNRIJWRKK-UHFFFAOYSA-N
Formula:	C12H22
SMILES:	CCCCC1=C(C)CCCC1
Mol. weight [g/mol]:	166.30

Physical Properties

Property code	Value	Unit	Source
gf	93.02	kJ/mol	Joback Method
hf	-181.51	kJ/mol	Joback Method
hfus	18.04	kJ/mol	Joback Method
hvap	44.66	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.457		Crippen Method
mcvol	164.780	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	165.50		NIST Webbook
tb	507.30	K	Joback Method
tc	703.95	K	Joback Method
tf	262.42	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.66	J/molxK	507.30	Joback Method
cpg	399.38	J/molxK	540.08	Joback Method
cpg	417.21	J/molxK	572.85	Joback Method
cpg	434.17	J/molxK	605.63	Joback Method
cpg	450.29	J/molxK	638.40	Joback Method
cpg	465.58	J/molxK	671.18	Joback Method
cpg	480.08	J/molxK	703.95	Joback Method
dvisc	0.0039283	Paxs	262.42	Joback Method
dvisc	0.0017166	Paxs	303.23	Joback Method

dvisc	0.0009130	Paxs	344.05	Joback Method
dvisc	0.0005551	Paxs	384.86	Joback Method
dvisc	0.0003713	Paxs	425.67	Joback Method
dvisc	0.0002665	Paxs	466.49	Joback Method
dvisc	0.0002017	Paxs	507.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R516600&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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