

Cyclopentene,1-heptyl-

Other names:	1-Heptyl-1-cyclopentene
Inchi:	InChI=1S/C12H22/c1-2-3-4-5-6-9-12-10-7-8-11-12/h10H,2-9,11H2,1H3
InchiKey:	FALRQTIXQCGLJF-UHFFFAOYSA-N
Formula:	C12H22
SMILES:	CCCCCCCC1=CCCC1
Mol. weight [g/mol]:	166.30
CAS:	4292-00-6

Physical Properties

Property code	Value	Unit	Source
gf	114.75	kJ/mol	Joback Method
hf	-163.88	kJ/mol	Joback Method
hfus	20.53	kJ/mol	Joback Method
hvap	43.83	kJ/mol	Joback Method
ie	8.41 ± 0.03	eV	NIST Webbook
log10ws	-4.59		Crippen Method
logp	4.457		Crippen Method
mcvol	164.780	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
ripol	1234.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1240.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1350.60		NIST Webbook
ripol	1354.60		NIST Webbook
ripol	1358.10		NIST Webbook
ripol	1362.20		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1368.60		NIST Webbook
ripol	1372.40		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1355.00		NIST Webbook

ripol	1351.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1365.60		NIST Webbook
tb	490.00 ± 15.00	K	NIST Webbook
tc	686.68	K	Joback Method
tf	253.42	K	Joback Method
vc	0.635	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.06	J/mol×K	498.05	Joback Method
cpg	397.16	J/mol×K	529.49	Joback Method
cpg	414.38	J/mol×K	560.93	Joback Method
cpg	430.74	J/mol×K	592.37	Joback Method
cpg	446.29	J/mol×K	623.80	Joback Method
cpg	461.04	J/mol×K	655.24	Joback Method
cpg	475.05	J/mol×K	686.68	Joback Method
dvisc	0.0042714	Paxs	253.42	Joback Method
dvisc	0.0019308	Paxs	294.19	Joback Method
dvisc	0.0010589	Paxs	334.96	Joback Method
dvisc	0.0006616	Paxs	375.74	Joback Method
dvisc	0.0004532	Paxs	416.51	Joback Method
dvisc	0.0003321	Paxs	457.28	Joback Method
dvisc	0.0002561	Paxs	498.05	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=C4292006&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
mccvol:	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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