

6-Heptenylcyclopentane

Inchi:	InChI=1S/C12H22/c1-2-3-4-5-6-9-12-10-7-8-11-12/h2,12H,1,3-11H2
InchiKey:	BPCUPKKBZIJNMGL-UHFFFAOYSA-N
Formula:	C12H22
SMILES:	C=CCCCCCC1CCCC1
Mol. weight [g/mol]:	166.30

Physical Properties

Property code	Value	Unit	Source
gf	174.55	kJ/mol	Joback Method
hf	-105.10	kJ/mol	Joback Method
hfus	19.49	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.313		Crippen Method
mvol	164.780	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1224.70		NIST Webbook
tb	485.92	K	Joback Method
tc	675.16	K	Joback Method
tf	234.14	K	Joback Method
vc	0.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.20	J/molxK	485.92	Joback Method
cpg	395.62	J/molxK	517.46	Joback Method
cpg	414.08	J/molxK	549.00	Joback Method
cpg	431.61	J/molxK	580.54	Joback Method
cpg	448.24	J/molxK	612.08	Joback Method
cpg	464.00	J/molxK	643.62	Joback Method
cpg	478.94	J/molxK	675.16	Joback Method
dvisc	0.0049306	Paxs	234.14	Joback Method
dvisc	0.0021396	Paxs	276.10	Joback Method

dvisc	0.0011573	Paxs	318.07	Joback Method
dvisc	0.0007224	Paxs	360.03	Joback Method
dvisc	0.0004975	Paxs	401.99	Joback Method
dvisc	0.0003677	Paxs	443.96	Joback Method
dvisc	0.0002863	Paxs	485.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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