Benzene, 1-hexenyl-, (E)

Inchi: InChI=1S/C12H16/c1-2-3-4-6-9-12-10-7-5-8-11-12/h5-11H,2-4H2,1H3/b9-6+
InchiKey: KETWBQOXTBGBBN-RMKNXTFCSA-N
Formula: C12H16
SMILES: CCCCC=Cc1ccccc1
Mol. weight [g/mol]: 160.26
CAS: 6111-82-6

Physical Properties

Property code	Value	Unit	Source
gf	242.79	kJ/mol	Joback Method
hf	62.74	kJ/mol	Joback Method
hfus	21.08	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.890		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1308.00		NIST Webbook
rinpol	1308.00		NIST Webbook
tb	504.80	K	Joback Method
tc	713.49	K	Joback Method
tf	246.34	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.28	J/mol×K	504.80	Joback Method
cpg	344.81	J/mol×K	539.58	Joback Method
cpg	360.34	J/mol×K	574.36	Joback Method
cpg	374.92	J/mol×K	609.14	Joback Method
cpg	388.61	J/mol×K	643.93	Joback Method
cpg	401.45	J/mol×K	678.71	Joback Method
cpg	413.50	J/mol×K	713.49	Joback Method

dvisc	0.0035637	Pa×s	246.34	Joback Method
dvisc	0.0014839	Pa×s	289.42	Joback Method
dvisc	0.0007754	Pa×s	332.49	Joback Method
dvisc	0.0004702	Pa×s	375.57	Joback Method
dvisc	0.0003160	Pa×s	418.65	Joback Method
dvisc	0.0002288	Pa×s	461.72	Joback Method
dvisc	0.0001750	Pa×s	504.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6111826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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