

Hex-1-enylbenzene

Other names:	1-phenyl-1-hexene
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:	828-15-9

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
tb	504.80	K	Joback Method
tc	713.49	K	Joback Method
tf	246.34	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.28	J/mol×K	504.80	Joback Method
cpg	401.45	J/mol×K	678.71	Joback Method
cpg	388.61	J/mol×K	643.93	Joback Method
cpg	374.92	J/mol×K	609.14	Joback Method
cpg	360.34	J/mol×K	574.36	Joback Method
cpg	344.81	J/mol×K	539.58	Joback Method
cpg	413.50	J/mol×K	713.49	Joback Method
dvisc	0.0001750	Paxs	504.80	Joback Method

dvisc	0.0002288	Paxs	461.72	Joback Method
dvisc	0.0003160	Paxs	418.65	Joback Method
dvisc	0.0004702	Paxs	375.57	Joback Method
dvisc	0.0007754	Paxs	332.49	Joback Method
dvisc	0.0014839	Paxs	289.42	Joback Method
dvisc	0.0035637	Paxs	246.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C828159&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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