

Benzene, (1-pentylhexyl)-

Other names:	Undecane, 6-phenyl-
Inchi:	InChI=1S/C17H28/c1-3-5-8-12-16(13-9-6-4-2)17-14-10-7-11-15-17/h7,10-11,14-16H,3-6,
InchiKey:	WCABIRIFXVGQH-UHFFFAOYSA-N
Formula:	C17H28
SMILES:	CCCCC(CCCCC)c1ccccc1
Mol. weight [g/mol]:	232.40
CAS:	4537-14-8

Physical Properties

Property code	Value	Unit	Source
gf	202.23	kJ/mol	Joback Method
hf	-162.96	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.931		Crippen Method
mcvol	226.630	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	278.10		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1625.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	614.60	K	Joback Method
tc	805.23	K	Joback Method
tf	292.77	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.76	J/mol×K	614.60	Joback Method
cpg	687.89	J/mol×K	773.46	Joback Method
cpg	671.98	J/mol×K	741.69	Joback Method

cpg	655.16	J/mol×K	709.91	Joback Method
cpg	637.37	J/mol×K	678.14	Joback Method
cpg	618.59	J/mol×K	646.37	Joback Method
cpg	702.92	J/mol×K	805.23	Joback Method
dvisc	0.0001273	Pa×s	614.60	Joback Method
dvisc	0.0001733	Pa×s	560.96	Joback Method
dvisc	0.0002518	Pa×s	507.32	Joback Method
dvisc	0.0003996	Pa×s	453.69	Joback Method
dvisc	0.0007180	Pa×s	400.05	Joback Method
dvisc	0.0015465	Pa×s	346.41	Joback Method
dvisc	0.0044125	Pa×s	292.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4537148&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
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
mcvol:	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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