

Benzene, (1-propyloctyl)-

Other names:	Undecane, 4-phenyl-
Inchi:	InChI=1S/C17H28/c1-3-5-6-7-9-13-16(12-4-2)17-14-10-8-11-15-17/h8,10-11,14-16H,3-7,
InchiKey:	NSQAXMRLBNXEHK-UHFFFAOYSA-N
Formula:	C17H28
SMILES:	CCCCCCCC(CCC)c1ccccc1
Mol. weight [g/mol]:	232.40
CAS:	4536-86-1

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	1645.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	280.20		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	280.20		NIST Webbook
ripol	1843.00		NIST Webbook
ripol	1843.00		NIST Webbook
tb	614.60	K	Joback Method
tc	805.23	K	Joback Method
tf	292.77	K	Joback Method
vc	0.874	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.76	J/molxK	614.60	Joback Method
cpg	618.59	J/molxK	646.37	Joback Method
cpg	637.37	J/molxK	678.14	Joback Method
cpg	655.16	J/molxK	709.91	Joback Method
cpg	671.98	J/molxK	741.69	Joback Method
cpg	687.89	J/molxK	773.46	Joback Method
cpg	702.92	J/molxK	805.23	Joback Method
dvisc	0.0044125	Paxs	292.77	Joback Method
dvisc	0.0015465	Paxs	346.41	Joback Method
dvisc	0.0007180	Paxs	400.05	Joback Method
dvisc	0.0003996	Paxs	453.69	Joback Method
dvisc	0.0002518	Paxs	507.32	Joback Method
dvisc	0.0001733	Paxs	560.96	Joback Method
dvisc	0.0001273	Paxs	614.60	Joback Method

Sources

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=C4536861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.cheméo.com/cid/19-421-3/Benzene-1-propyloctyl.pdf>

Generated by Cheméo on 2024-04-17 17:52:03.977678453 +0000 UTC m=+15665572.898255768.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.