

Benzene, 1-ethyl-2-hexyl

Inchi:	InChI=1S/C14H22/c1-3-5-6-7-11-14-12-9-8-10-13(14)4-2/h8-10,12H,3-7,11H2,1-2H3
InchiKey:	XMTLOBXRRJCFFJ-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	CCCCCc1ccccc1CC
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	169.78	kJ/mol	Joback Method
hf	-107.23	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.372		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1398.00		NIST Webbook
rinpol	1398.00		NIST Webbook
tb	551.38	K	Joback Method
tc	746.43	K	Joback Method
tf	286.48	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.44	J/molxK	551.38	Joback Method
cpg	460.30	J/molxK	583.89	Joback Method
cpg	477.25	J/molxK	616.40	Joback Method
cpg	493.33	J/molxK	648.91	Joback Method
cpg	508.57	J/molxK	681.42	Joback Method
cpg	522.99	J/molxK	713.92	Joback Method
cpg	536.64	J/molxK	746.43	Joback Method
dvisc	0.0026153	Paxs	286.48	Joback Method

dvisc	0.0012344	Paxs	330.63	Joback Method
dvisc	0.0006953	Paxs	374.78	Joback Method
dvisc	0.0004420	Paxs	418.93	Joback Method
dvisc	0.0003064	Paxs	463.08	Joback Method
dvisc	0.0002263	Paxs	507.23	Joback Method
dvisc	0.0001755	Paxs	551.38	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=R13660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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