1-METHYL-2-N-HEXYLBENZENE

Other names: Benzene, 1-hexyl-2-methyl
Benzene, 1-methyl-2-hexyl
Inchi: InChI=1S/C13H20/c1-3-4-5-6-10-13-11-8-7-9-12(13)2/h7-9,11H,3-6,10H2,1-2H3
InchiKey: BNXNQXKAEVKUJG-UHFFFAOYSA-N
Formula: C13H20
SMILES: CCCCCCc1ccccc1C
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
af	0.5135		Cheméo Relay (1.0)
gf	161.36	kJ/mol	Joback Method
hf	-74.73	kJ/mol	Cheméo Relay (1.0)
hfus	23.08	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-5.29		Cheméo Relay (1.0)
logp	4.118		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1622.00		NIST Webbook
tb	518.39	K	Cheméo Relay (1.0)
tc	709.39	K	Cheméo Relay (1.0)
tf	233.62	K	Cheméo Relay (1.0)
vc	0.649	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.45	J/mol×K	528.50	Joback Method
cpg	410.68	J/mol×K	561.45	Joback Method
cpg	427.04	J/mol×K	594.40	Joback Method
cpg	442.55	J/mol×K	627.35	Joback Method
cpg	457.24	J/mol×K	660.30	Joback Method
cpg	471.14	J/mol×K	693.25	Joback Method
cpg	484.29	J/mol×K	726.20	Joback Method
dvisc	0.0026431	Pa×s	275.21	Joback Method
dvisc	0.0012700	Pa×s	317.42	Joback Method
dvisc	0.0007248	Pa×s	359.64	Joback Method
dvisc	0.0004654	Pa×s	401.86	Joback Method
dvisc	0.0003251	Pa×s	444.07	Joback Method
dvisc	0.0002417	Pa×s	486.28	Joback Method
dvisc	0.0001884	Pa×s	528.50	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1595104&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

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
ie:	Ionization energy
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