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
CAS: 1595-10-4

Physical Properties

Property code	Value	Unit	Source
gf	161.36	kJ/mol	Joback Method
hf	-86.59	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
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	1622.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1636.00		NIST Webbook
tb	528.50	K	Joback Method
tc	726.20	K	Joback Method
tf	275.21	K	Joback Method
vc	0.655	m3/kmol	Joback Method

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

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=C1595104&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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