1-METHYL-4-N-HEXYLBENZENE

Other names: Benzene, 1-hexyl-4-methyl
Benzene, 1-methyl-4-hexyl
Inchi: InChI=1S/C13H20/c1-3-4-5-6-7-13-10-8-12(2)9-11-13/h8-11H,3-7H2,1-2H3
InchiKey: BCJOBVWKIGRZCW-UHFFFAOYSA-N
Formula: C13H20
SMILES: CCCCCCc1ccc(C)cc1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
af	0.5323		Cheméo Relay (1.0)
gf	161.36	kJ/mol	Joback Method
hf	-77.30	kJ/mol	Cheméo Relay (1.0)
hfus	23.08	kJ/mol	Joback Method
hvap	62.51	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-5.38		Cheméo Relay (1.0)
logp	4.118		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1333.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1579.60		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1601.00		NIST Webbook
tb	518.86	K	Cheméo Relay (1.0)
tc	704.57	K	Cheméo Relay (1.0)
tf	242.70 ± 1.00	K	NIST Webbook
vc	0.659	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	484.29	J/mol×K	726.20	Joback Method
cpg	471.14	J/mol×K	693.25	Joback Method
cpg	457.24	J/mol×K	660.30	Joback Method
cpg	442.55	J/mol×K	627.35	Joback Method
cpg	427.04	J/mol×K	594.40	Joback Method
cpg	410.68	J/mol×K	561.45	Joback Method
dvisc	0.0004654	Pa×s	401.86	Joback Method
dvisc	0.0001884	Pa×s	528.50	Joback Method
dvisc	0.0002417	Pa×s	486.28	Joback Method
dvisc	0.0003251	Pa×s	444.07	Joback Method
dvisc	0.0026431	Pa×s	275.21	Joback Method
dvisc	0.0007248	Pa×s	359.64	Joback Method
dvisc	0.0012700	Pa×s	317.42	Joback Method

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1595013&Units=SI

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