

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
CAS:	1595-01-3

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
ripol	1333.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1579.60		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1571.00		NIST Webbook
tb	528.50	K	Joback Method
tc	726.20	K	Joback Method
tf	242.70 ± 1.00	K	NIST Webbook
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1595013&Units=SI

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

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