Benzene, (1-ethylbutyl)-

Other names:	(1-Ethylbutyl)benzene
	(3-Hexyl)benzene
	3-Phenylhexane
	Hexane, 3-phenyl-
Inchi:	InChI=1S/C12H18/c1-3-8-11(4-2)12-9-6-5-7-10-12/h5-7,9-11H,3-4,8H2,1-2H3
InchiKey:	SLVCCWGFGQVDMN-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCCC(CC)c1ccccc1
Mol. weight [g/mol]:	162.27
CAS:	4468-42-2

Physical Properties

Property code	Value	Unit	Source
chl	-6757.00	kJ/mol	NIST Webbook
gf	160.13	kJ/mol	Joback Method
hf	-59.76	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.980		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
ripol	1352.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1352.40		NIST Webbook
tb	481.40 ± 0.20	K	NIST Webbook
tb	474.90 ± 4.00	K	NIST Webbook
tb	483.00 ± 2.00	K	NIST Webbook
tc	703.92	K	Joback Method
tf	217.78 ± 0.20	K	NIST Webbook
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.64	J/mol×K	500.20	Joback Method
cpg	362.97	J/mol×K	534.15	Joback Method
cpg	379.35	J/mol×K	568.11	Joback Method
cpg	394.81	J/mol×K	602.06	Joback Method
cpg	409.40	J/mol×K	636.01	Joback Method
cpg	423.14	J/mol×K	669.96	Joback Method
cpg	436.08	J/mol×K	703.92	Joback Method
dvisc	0.0057131	Pa×s	236.42	Joback Method
dvisc	0.0020964	Pa×s	280.38	Joback Method
dvisc	0.0010095	Pa×s	324.35	Joback Method
dvisc	0.0005788	Pa×s	368.31	Joback Method
dvisc	0.0003736	Pa×s	412.27	Joback Method
dvisc	0.0002624	Pa×s	456.24	Joback Method
dvisc	0.0001961	Pa×s	500.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47422e+01
Coeff. B	-4.12002e+03
Coeff. C	-7.51880e+01
Temperature range (K), min.	360.22
Temperature range (K), max.	512.06

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4468422&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume