

Benzene, 1-ethyl-3-butyl

Other names:	1-Ethyl-3-n-Butylbenzene
Inchi:	InChI=1S/C12H18/c1-3-5-7-12-9-6-8-11(4-2)10-12/h6,8-10H,3-5,7H2,1-2H3
InchiKey:	IBQJOCAGNFEEKY-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCCCc1cccc(CC)c1
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	152.94	kJ/mol	Joback Method
hf	-65.95	kJ/mol	Joback Method
hfus	20.49	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.592		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
ripol	1423.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1422.60		NIST Webbook
tb	505.62	K	Joback Method
tc	706.05	K	Joback Method
tf	263.94	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.19	J/mol×K	505.62	Joback Method
cpg	420.54	J/mol×K	672.64	Joback Method
cpg	407.24	J/mol×K	639.24	Joback Method
cpg	393.19	J/mol×K	605.83	Joback Method
cpg	378.35	J/mol×K	572.43	Joback Method
cpg	362.69	J/mol×K	539.02	Joback Method

cpg	433.10	J/mol×K	706.05	Joback Method
dvisc	0.0002000	Pa×s	505.62	Joback Method
dvisc	0.0002551	Pa×s	465.34	Joback Method
dvisc	0.0003409	Pa×s	425.06	Joback Method
dvisc	0.0004839	Pa×s	384.78	Joback Method
dvisc	0.0007455	Pa×s	344.50	Joback Method
dvisc	0.0012879	Pa×s	304.22	Joback Method
dvisc	0.0026290	Pa×s	263.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R52975&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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