Benzene, 1-butyl-4-ethyl

Other names: 1-Ethyl-4-n-Butylbenzene
Inchi: InChI=1S/C12H18/c1-3-5-6-12-9-7-11(4-2)8-10-12/h7-10H,3-6H2,1-2H3
InchiKey: UPYBAFFRUZTWFA-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCCCc1ccc(CC)cc1
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
rinpol	1231.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1227.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1470.30		NIST Webbook
ripol	1439.50		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1470.30		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

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=R12462&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