Benzene, 1-butyl-2,4-dimethyl

Other names: 1,3-Dimethyl-4-n-Butylbenzene
Inchi: InChI=1S/C12H18/c1-4-5-6-12-8-7-10(2)9-11(12)3/h7-9H,4-6H2,1-3H3
InchiKey: JEHCWPAYIBNVDI-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCCCc1ccc(C)cc1C
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	143.31	kJ/mol	Joback Method
hf	-77.42	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	45.91	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.646		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1249.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1487.30		NIST Webbook
ripol	1487.00		NIST Webbook
tb	510.60	K	Joback Method
tc	712.18	K	Joback Method
tf	276.46	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.80	J/mol×K	510.60	Joback Method

cpg	362.94	J/mol×K	544.20	Joback Method
cpg	378.30	J/mol×K	577.79	Joback Method
cpg	392.88	J/mol×K	611.39	Joback Method
cpg	406.73	J/mol×K	644.99	Joback Method
cpg	419.85	J/mol×K	678.59	Joback Method
cpg	432.28	J/mol×K	712.18	Joback Method
dvisc	0.0018797	Pa×s	276.46	Joback Method
dvisc	0.0010177	Pa×s	315.48	Joback Method
dvisc	0.0006307	Pa×s	354.51	Joback Method
dvisc	0.0004298	Pa×s	393.53	Joback Method
dvisc	0.0003139	Pa×s	432.55	Joback Method
dvisc	0.0002414	Pa×s	471.58	Joback Method
dvisc	0.0001933	Pa×s	510.60	Joback Method

Sources

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=R52939&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