Benzene, 1,4-dibutyl

Other names: 1,4-Di-n-butylbenzene
Inchi: InChI=1S/C14H22/c1-3-5-7-13-9-11-14(12-10-13)8-6-4-2/h9-12H,3-8H2,1-2H3
InchiKey: VGQOZYOOFXEGDA-UHFFFAOYSA-N
Formula: C14H22
SMILES: CCCCc1ccc(CCCC)cc1
Mol. weight [g/mol]: 190.32
CAS: 1571-86-4

Physical Properties

Property code	Value	Unit	Source
gf	169.78	kJ/mol	Joback Method
hf	-107.23	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
log10ws	-4.75		Crippen Method
logp	4.372		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1411.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1640.30		NIST Webbook
ripol	1640.30		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1631.00		NIST Webbook
tb	509.20	K	NIST Webbook
tc	746.43	K	Joback Method
tf	179.00 ± 6.00	K	NIST Webbook
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.44	J/mol×K	551.38	Joback Method

cpg	460.30	J/mol×K	583.89	Joback Method
cpg	477.25	J/mol×K	616.40	Joback Method
cpg	493.33	J/mol×K	648.91	Joback Method
cpg	508.57	J/mol×K	681.42	Joback Method
cpg	522.99	J/mol×K	713.92	Joback Method
cpg	536.64	J/mol×K	746.43	Joback Method
dvisc	0.0026153	Pa×s	286.48	Joback Method
dvisc	0.0012344	Pa×s	330.63	Joback Method
dvisc	0.0006953	Pa×s	374.78	Joback Method
dvisc	0.0004420	Pa×s	418.93	Joback Method
dvisc	0.0003064	Pa×s	463.08	Joback Method
dvisc	0.0002263	Pa×s	507.23	Joback Method
dvisc	0.0001755	Pa×s	551.38	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1571864&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
ie: Ionization energy
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