Benzene, 1-butyl-3-(1-methylpropyl)

Inchi: InChI=1S/C14H22/c1-4-6-8-13-9-7-10-14(11-13)12(3)5-2/h7,9-12H,4-6,8H2,1-3H3
InchiKey: LEXMLNFPCCTVIF-UHFFFAOYSA-N
Formula: C14H22
SMILES: CCCCc1cccc(C(C)CC)c1
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	167.34	kJ/mol	Joback Method
hf	-112.51	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.543		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
ripol	1514.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1526.00		NIST Webbook
tb	550.94	K	Joback Method
tc	750.04	K	Joback Method
tf	271.48	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.71	J/mol×K	550.94	Joback Method
cpg	461.01	J/mol×K	584.12	Joback Method
cpg	478.35	J/mol×K	617.31	Joback Method
cpg	494.77	J/mol×K	650.49	Joback Method

cpg	510.30	J/mol×K	683.67	Joback Method
cpg	524.99	J/mol×K	716.85	Joback Method
cpg	538.86	J/mol×K	750.04	Joback Method
dvisc	0.0035872	Pa×s	271.48	Joback Method
dvisc	0.0014741	Pa×s	318.06	Joback Method
dvisc	0.0007603	Pa×s	364.63	Joback Method
dvisc	0.0004556	Pa×s	411.21	Joback Method
dvisc	0.0003030	Pa×s	457.79	Joback Method
dvisc	0.0002173	Pa×s	504.36	Joback Method
dvisc	0.0001648	Pa×s	550.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R550071&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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