Benzene, 1-butyl-4-(1,1-dimethylethyl)

Inchi: InChI=1S/C14H22/c1-5-6-7-12-8-10-13(11-9-12)14(2,3)4/h8-11H,5-7H2,1-4H3
InchiKey: BDSMPLDBKOVNHW-UHFFFAOYSA-N
Formula: C14H22
SMILES: CCCCc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	172.62	kJ/mol	Joback Method
hf	-115.98	kJ/mol	Joback Method
hfus	18.25	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.327		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1345.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1566.50		NIST Webbook
ripol	1559.00		NIST Webbook
tb	548.15	K	Joback Method
tc	755.00	K	Joback Method
tf	288.90	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.34	J/mol×K	548.15	Joback Method
cpg	529.73	J/mol×K	720.53	Joback Method
cpg	514.89	J/mol×K	686.05	Joback Method
cpg	499.08	J/mol×K	651.58	Joback Method
cpg	482.26	J/mol×K	617.10	Joback Method
cpg	464.37	J/mol×K	582.63	Joback Method

cpg	543.67	J/mol×K	755.00	Joback Method
dvisc	0.0001624	Pa×s	548.15	Joback Method
dvisc	0.0002168	Pa×s	504.94	Joback Method
dvisc	0.0003055	Pa×s	461.73	Joback Method
dvisc	0.0004621	Pa×s	418.52	Joback Method
dvisc	0.0007690	Pa×s	375.32	Joback Method
dvisc	0.0014610	Pa×s	332.11	Joback Method
dvisc	0.0033632	Pa×s	288.90	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R12551&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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