Benzene, 1-sec-butyl-4-isobutyl

Inchi: InChI=1S/C15H24/c1-5-13(4)15-10-8-14(9-11-15)7-6-12(2)3/h8-13H,5-7H2,1-4H3
InchiKey: PDOUOUPXZUDSOM-UHFFFAOYSA-N
Formula: C15H24
SMILES: CCC(C)c1ccc(CCC(C)C)cc1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	173.32	kJ/mol	Joback Method
hf	-138.43	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	51.15	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.789		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
ripol	1494.00		NIST Webbook
ripol	1494.00		NIST Webbook
tb	573.38	K	Joback Method
tc	773.72	K	Joback Method
tf	267.75	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.68	J/mol×K	573.38	Joback Method
cpg	512.93	J/mol×K	606.77	Joback Method
cpg	531.15	J/mol×K	640.16	Joback Method
cpg	548.39	J/mol×K	673.55	Joback Method
cpg	564.68	J/mol×K	706.94	Joback Method
cpg	580.06	J/mol×K	740.33	Joback Method
cpg	594.57	J/mol×K	773.72	Joback Method
dvisc	0.0049185	Pa×s	267.75	Joback Method

dvisc	0.0016990	Pa×s	318.69	Joback Method
dvisc	0.0007866	Pa×s	369.63	Joback Method
dvisc	0.0004389	Pa×s	420.56	Joback Method
dvisc	0.0002778	Pa×s	471.50	Joback Method
dvisc	0.0001922	Pa×s	522.44	Joback Method
dvisc	0.0001420	Pa×s	573.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R549061&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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