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

Inchi: InChI=1S/C13H20/c1-10(2)11-6-8-12(9-7-11)13(3,4)5/h6-10H,1-5H3
InchiKey: QLPNXSSDHYYKBS-UHFFFAOYSA-N
Formula: C13H20
SMILES: CC(C)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	161.76	kJ/mol	Joback Method
hf	-100.62	kJ/mol	Joback Method
hfus	12.14	kJ/mol	Joback Method
hvap	45.79	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	4.107		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
ripol	1460.00		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1462.00		NIST Webbook
ripol	1472.00		NIST Webbook
ripol	1487.00		NIST Webbook
tb	524.83	K	Joback Method
tc	739.67	K	Joback Method
tf	262.63	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.59	J/mol×K	524.83	Joback Method
cpg	480.24	J/mol×K	703.86	Joback Method
cpg	465.63	J/mol×K	668.05	Joback Method
cpg	450.02	J/mol×K	632.25	Joback Method

cpg	433.35	J/mol×K	596.44	Joback Method
cpg	415.56	J/mol×K	560.64	Joback Method
cpg	493.91	J/mol×K	739.67	Joback Method
dvisc	0.0001675	Pa×s	524.83	Joback Method
dvisc	0.0002285	Pa×s	481.13	Joback Method
dvisc	0.0003317	Pa×s	437.43	Joback Method
dvisc	0.0005231	Pa×s	393.73	Joback Method
dvisc	0.0009242	Pa×s	350.03	Joback Method
dvisc	0.0019209	Pa×s	306.33	Joback Method
dvisc	0.0050928	Pa×s	262.63	Joback Method

Sources

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=R555927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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