Benzene, 2-(1,1-dimethylethyl)-1,4-dimethyl

Inchi: InChI=1S/C12H18/c1-9-6-7-10(2)11(8-9)12(3,4)5/h6-8H,1-5H3
InchiKey: IRMLULIFOFYBTI-UHFFFAOYSA-N
Formula: C12H18
SMILES: Cc1ccc(C)c(C(C)(C)C)c1
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	146.15	kJ/mol	Joback Method
hf	-86.17	kJ/mol	Joback Method
hfus	12.69	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.601		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1164.00		NIST Webbook
tb	507.37	K	Joback Method
tc	722.03	K	Joback Method
tf	278.88	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.74	J/mol×K	507.37	Joback Method
cpg	426.96	J/mol×K	686.25	Joback Method
cpg	413.40	J/mol×K	650.48	Joback Method
cpg	398.95	J/mol×K	614.70	Joback Method
cpg	383.55	J/mol×K	578.92	Joback Method
cpg	367.17	J/mol×K	543.15	Joback Method
cpg	439.68	J/mol×K	722.03	Joback Method
dvisc	0.0001852	Pa×s	507.37	Joback Method
dvisc	0.0002397	Pa×s	469.29	Joback Method

dvisc	0.0003246	Pa×s	431.21	Joback Method
dvisc	0.0004663	Pa×s	393.12	Joback Method
dvisc	0.0007238	Pa×s	355.04	Joback Method
dvisc	0.0012488	Pa×s	316.96	Joback Method
dvisc	0.0025008	Pa×s	278.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R53123&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume