

Benzene, 1,2-dimethyl-4,5-bis-(1-methylethyl)

Inchi:	InChI=1S/C14H22/c1-9(2)13-7-11(5)12(6)8-14(13)10(3)4/h7-10H,1-6H3
InchiKey:	WGWYYHMLBYHLKK-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	Cc1cc(C(C)C)c(C(C)C)cc1C
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	145.64	kJ/mol	Joback Method
hf	-140.73	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	50.24	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.550		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
ripol	1586.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	560.46	K	Joback Method
tc	765.83	K	Joback Method
tf	281.52	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.88	J/mol×K	560.46	Joback Method
cpg	525.82	J/mol×K	731.60	Joback Method

cpg	511.14	J/mol×K	697.37	Joback Method
cpg	495.64	J/mol×K	663.14	Joback Method
cpg	479.27	J/mol×K	628.92	Joback Method
cpg	462.03	J/mol×K	594.69	Joback Method
cpg	539.70	J/mol×K	765.83	Joback Method
dvisc	0.0001473	Pa×s	560.46	Joback Method
dvisc	0.0001902	Pa×s	513.97	Joback Method
dvisc	0.0002584	Pa×s	467.48	Joback Method
dvisc	0.0003757	Pa×s	420.99	Joback Method
dvisc	0.0005993	Pa×s	374.50	Joback Method
dvisc	0.0010915	Pa×s	328.01	Joback Method
dvisc	0.0024229	Pa×s	281.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R555952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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