

Benzene, 2-methyl-1,4-bis(1-methylethyl)-

Other names:	1,4-Diisopropyl-2-methylbenzene
Inchi:	InChI=1S/C13H20/c1-9(2)12-6-7-13(10(3)4)11(5)8-12/h6-10H,1-5H3
InchiKey:	BRXCOIOOGGCKPZ-UHFFFAOYSA-N
Formula:	C13H20
SMILES:	<chem>Cc1cc(C(C)C)ccc1C(C)C</chem>
Mol. weight [g/mol]:	176.30
CAS:	58502-85-5

Physical Properties

Property code	Value	Unit	Source
gf	146.85	kJ/mol	Joback Method
hf	-108.62	kJ/mol	Joback Method
hfus	15.64	kJ/mol	Joback Method
hvap	47.36	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.242		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1210.00		NIST Webbook
tb	532.60	K	Joback Method
tc	740.08	K	Joback Method
tf	257.73	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.49	J/molxK	532.60	Joback Method
cpg	412.29	J/molxK	567.18	Joback Method
cpg	429.16	J/molxK	601.76	Joback Method
cpg	445.14	J/molxK	636.34	Joback Method
cpg	460.25	J/molxK	670.92	Joback Method
cpg	474.53	J/molxK	705.50	Joback Method
cpg	488.00	J/molxK	740.08	Joback Method

dvisc	0.0035478	Paxs	257.73	Joback Method
dvisc	0.0014389	Paxs	303.54	Joback Method
dvisc	0.0007394	Paxs	349.35	Joback Method
dvisc	0.0004434	Paxs	395.17	Joback Method
dvisc	0.0002957	Paxs	440.98	Joback Method
dvisc	0.0002128	Paxs	486.79	Joback Method
dvisc	0.0001621	Paxs	532.60	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=C58502855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	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

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