

1,3-Dimethyl-4-isobutylbenzene

Inchi:	InChI=1S/C12H18/c1-9(2)7-12-6-5-10(3)8-11(12)4/h5-6,8-9H,7H2,1-4H3
InchiKey:	KYPUBILZJUPGAD-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	<chem>Cc1ccc(CC(C)C)c(C)c1</chem>
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	140.87	kJ/mol	Joback Method
hf	-82.70	kJ/mol	Joback Method
hfus	16.58	kJ/mol	Joback Method
hvap	45.52	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.502		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
ripol	1400.80		NIST Webbook
ripol	1400.80		NIST Webbook
tb	510.16	K	Joback Method
tc	716.23	K	Joback Method
tf	261.46	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.02	J/molxK	510.16	Joback Method
cpg	421.81	J/molxK	681.89	Joback Method
cpg	408.42	J/molxK	647.54	Joback Method
cpg	394.28	J/molxK	613.20	Joback Method
cpg	379.34	J/molxK	578.85	Joback Method
cpg	363.60	J/molxK	544.51	Joback Method
cpg	434.46	J/molxK	716.23	Joback Method
dvisc	0.0001825	Paxs	510.16	Joback Method

dvisc	0.0002330	Paxs	468.71	Joback Method
dvisc	0.0003119	Paxs	427.26	Joback Method
dvisc	0.0004446	Paxs	385.81	Joback Method
dvisc	0.0006900	Paxs	344.36	Joback Method
dvisc	0.0012079	Paxs	302.91	Joback Method
dvisc	0.0025252	Paxs	261.46	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=R305618&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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