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: Cc1ccc(CC(C)C)c(C)c1
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/mol×K	510.16	Joback Method
cpg	363.60	J/mol×K	544.51	Joback Method
cpg	379.34	J/mol×K	578.85	Joback Method
cpg	394.28	J/mol×K	613.20	Joback Method
cpg	408.42	J/mol×K	647.54	Joback Method
cpg	421.81	J/mol×K	681.89	Joback Method
cpg	434.46	J/mol×K	716.23	Joback Method
dvisc	0.0025252	Pa×s	261.46	Joback Method

dvisc	0.0012079	Pa×s	302.91	Joback Method
dvisc	0.0006900	Pa×s	344.36	Joback Method
dvisc	0.0004446	Pa×s	385.81	Joback Method
dvisc	0.0003119	Pa×s	427.26	Joback Method
dvisc	0.0002330	Pa×s	468.71	Joback Method
dvisc	0.0001825	Pa×s	510.16	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/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

Latest version available from:
https://www.chemeo.com/cid/75-524-7/1-3-Dimethyl-4-isobutylbenzene.pdf
Generated by Cheméo on 2024-10-12 04:44:56.640646498 +0000 UTC m=+3289159.277615746.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.