

1,3-Dimethyl-4-cyclohexylbenzene

Other names:	1-cyclohexyl-2,4-dimethylbenzene
Inchi:	InChI=1S/C14H20/c1-11-8-9-14(12(2)10-11)13-6-4-3-5-7-13/h8-10,13H,3-7H2,1-2H3
InchiKey:	AGLWOTGIKIGSJD-UHFFFAOYSA-N
Formula:	C14H20
SMILES:	<chem>Cc1ccc(C2CCCCC2)c(C)c1</chem>
Mol. weight [g/mol]:	188.31
CAS:	4501-51-3

Physical Properties

Property code	Value	Unit	Source
gf	184.60	kJ/mol	Joback Method
hf	-64.38	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	50.79	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.351		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
tb	575.91	K	Joback Method
tc	809.50	K	Joback Method
tf	306.38	K	Joback Method
vc	0.644	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.19	J/molxK	575.91	Joback Method
cpg	454.81	J/molxK	614.84	Joback Method
cpg	475.04	J/molxK	653.77	Joback Method
cpg	493.94	J/molxK	692.70	Joback Method
cpg	511.55	J/molxK	731.64	Joback Method
cpg	527.94	J/molxK	770.57	Joback Method
cpg	543.13	J/molxK	809.50	Joback Method
dvisc	0.0024420	Paxs	306.38	Joback Method

dvisc	0.0012093	Paxs	351.30	Joback Method
dvisc	0.0007023	Paxs	396.22	Joback Method
dvisc	0.0004556	Paxs	441.14	Joback Method
dvisc	0.0003202	Paxs	486.07	Joback Method
dvisc	0.0002388	Paxs	530.99	Joback Method
dvisc	0.0001865	Paxs	575.91	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=C4501513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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