

Benzene, 1-cyclohexyl-3-methyl-

Other names:	Toluene, m-cyclohexyl- m-Cyclohexyltoluene
Inchi:	InChI=1S/C13H18/c1-11-6-5-9-13(10-11)12-7-3-2-4-8-12/h5-6,9-10,12H,2-4,7-8H2,1H3
InchiKey:	ULBWADKCMNAMFJ-UHFFFAOYSA-N
Formula:	C13H18
SMILES:	<chem>Cc1cccc(C2CCCCC2)c1</chem>
Mol. weight [g/mol]:	174.28
CAS:	4575-46-6

Physical Properties

Property code	Value	Unit	Source
gf	185.81	kJ/mol	Joback Method
hf	-32.27	kJ/mol	Joback Method
hfus	14.91	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.043		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	548.05	K	Joback Method
tc	785.26	K	Joback Method
tf	282.59	K	Joback Method
vc	0.589	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.33	J/mol×K	548.05	Joback Method
cpg	403.84	J/mol×K	587.59	Joback Method
cpg	423.91	J/mol×K	627.12	Joback Method
cpg	442.60	J/mol×K	666.66	Joback Method
cpg	459.99	J/mol×K	706.19	Joback Method
cpg	476.11	J/mol×K	745.73	Joback Method
cpg	491.03	J/mol×K	785.26	Joback Method

dvisc	0.0034256	Paxs	282.59	Joback Method
dvisc	0.0015608	Paxs	326.83	Joback Method
dvisc	0.0008578	Paxs	371.08	Joback Method
dvisc	0.0005355	Paxs	415.32	Joback Method
dvisc	0.0003661	Paxs	459.56	Joback Method
dvisc	0.0002676	Paxs	503.81	Joback Method
dvisc	0.0002057	Paxs	548.05	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=C4575466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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