

o-Cymene

Other names:	1-(1-methylethyl)-2-methylbenzene 1-Isopropyl-2-methylbenzene 1-Methyl-2-(1-methylethyl)-benzene 1-Methyl-2-iso-propylbenzene 1-Methyl-2-isopropylbenzene 1-methyl,2-n-isopropylbenzene 1-methyl-2-propan-2-ylbenzene 2-Isopropyltoluene Benzene, 1-methyl-2-(1-methylethyl)- Cymene, ortho UN 2046 o-Cymol o-Isopropyltoluene ortho-Cymene
Inchi:	InChI=1S/C10H14/c1-8(2)10-7-5-4-6-9(10)3/h4-8H,1-3H3
InchiKey:	WWRCMNKATXZARA-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	Cc1ccccc1C(C)C
Mol. weight [g/mol]:	134.22
CAS:	527-84-4

Physical Properties

Property code	Value	Unit	Source
chl	-5859.90 ± 2.20	kJ/mol	NIST Webbook
chl	-5862.62 ± 0.84	kJ/mol	NIST Webbook
gf	133.66	kJ/mol	Joback Method
hf	-29.95	kJ/mol	Joback Method
hfl	-76.10 ± 2.10	kJ/mol	NIST Webbook
hfl	-73.30 ± 1.00	kJ/mol	NIST Webbook
hfus	11.79	kJ/mol	Joback Method
hvap	50.60	kJ/mol	NIST Webbook
log10ws	-3.76		Estimated Solubility Method
log10ws	-3.76		Aqueous Solubility Prediction Method
logp	3.118		Crippen Method
mcvol	128.000	ml/mol	McGowan Method

pc	2909.25	kPa	Joback Method
rinpol	1022.00		NIST Webbook
rinpol	1013.50		NIST Webbook
rinpol	1032.30		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1028.00		NIST Webbook
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rinpol	1024.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1010.42		NIST Webbook
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rinpol	1033.00		NIST Webbook

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ripol	1254.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1274.80		NIST Webbook
tb	459.42	K	Joback Method
tc	670.22	K	Joback Method
tf	201.40	K	Aqueous Solubility Prediction Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.48	J/mol×K	670.22	Joback Method
cpg	325.13	J/mol×K	635.09	Joback Method
cpg	313.10	J/mol×K	599.96	Joback Method

cpg	300.33	J/mol×K	564.82	Joback Method
cpg	286.82	J/mol×K	529.69	Joback Method
cpg	272.52	J/mol×K	494.55	Joback Method
cpg	257.41	J/mol×K	459.42	Joback Method
dvisc	0.0035598	Pa×s	226.40	Joback Method
dvisc	0.0002060	Pa×s	459.42	Joback Method
dvisc	0.0002660	Pa×s	420.58	Joback Method
dvisc	0.0003618	Pa×s	381.75	Joback Method
dvisc	0.0005277	Pa×s	342.91	Joback Method
dvisc	0.0008475	Pa×s	304.07	Joback Method
dvisc	0.0015637	Pa×s	265.24	Joback Method
hvapt	44.40	kJ/mol	403.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.51654e+01
Coeff. B	-8.25896e+03
Coeff. C	-8.66782e+00
Coeff. D	3.57058e-06
Temperature range (K), min.	201.64
Temperature range (K), max.	662.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol672.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C527844&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=672
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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