

Benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-

Other names:	Anisole, 2-isopropyl-5-methyl- Methyl thymyl ether Thymol methyl ether Thymyl methyl ether 3-Methoxy-p-cymene 4-Isopropyl-3-methoxytoluene O-Methylthymol Methyl thymol ether 1-Isopropyl-2-methoxy-4-methylbenzene Methylthymol Thymol Me ether Thymol methyl 2-Isopropyl-5-methylanisole Thymyl methyl oxide Thymol methyl ether (=methyl thymol) Methyl thymyl oxide
Inchi:	InChI=1S/C11H16O/c1-8(2)10-6-5-9(3)7-11(10)12-4/h5-8H,1-4H3
InchiKey:	LSQXNMXDFRRDSJ-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	<chem>COc1cc(C)ccc1C(C)C</chem>
Mol. weight [g/mol]:	164.24
CAS:	1076-56-8

Physical Properties

Property code	Value	Unit	Source
gf	27.45	kJ/mol	Joback Method
hf	-194.28	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	45.70	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.127		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1235.00		NIST Webbook
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ripol	1611.00		NIST Webbook
ripol	1579.00		NIST Webbook
tb	509.70	K	Joback Method
tc	716.96	K	Joback Method
tf	272.42	K	Joback Method
vc	0.555	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.70	J/molxK	509.70	Joback Method
cpg	396.29	J/molxK	682.41	Joback Method
cpg	383.76	J/molxK	647.87	Joback Method
cpg	370.54	J/molxK	613.33	Joback Method
cpg	356.63	J/molxK	578.79	Joback Method
cpg	342.03	J/molxK	544.24	Joback Method
cpg	408.15	J/molxK	716.96	Joback Method
dvisc	0.0001623	Paxs	509.70	Joback Method
dvisc	0.0002057	Paxs	470.15	Joback Method
dvisc	0.0002723	Paxs	430.61	Joback Method
dvisc	0.0003817	Paxs	391.06	Joback Method
dvisc	0.0005771	Paxs	351.51	Joback Method
dvisc	0.0009689	Paxs	311.97	Joback Method
dvisc	0.0018910	Paxs	272.42	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=C1076568&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
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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