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

Other names: 2-Isopropyl-1-methoxy-4-methylbenzene
Isothymol methyl ether
Anisole, 2-isopropyl-4-methyl-
2-isopropyl-4-methylanisole

Inchi: InChI=1S/C11H16O/c1-8(2)10-7-9(3)5-6-11(10)12-4/h5-8H,1-4H3

InchiKey: CVUAHQAQHICPSF-UHFFFAOYSA-N

Formula: C11H16O

SMILES: COc1ccc(C)cc1C(C)C

Mol. weight [g/mol]: 164.24

CAS: 31574-44-4

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	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1215.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1595.00		NIST Webbook
tb	509.70	K	Joback Method
tc	716.96	K	Joback Method
tf	272.42	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31574444&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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