

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

Other names:	Anisole, 2-tert-butyl-5-methyl- 1-tert-Butyl-2-Methoxy-4-methylbenzene 2-tert-Butyl-5-Methylanisole 6-tert-Butyl-3-Methylanisole
Inchi:	InChI=1S/C12H18O/c1-9-6-7-10(12(2,3)4)11(8-9)13-5/h6-8H,1-5H3
InchiKey:	NFDFFEFJTYRAHEM-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	COc1cc(C)ccc1C(C)(C)C
Mol. weight [g/mol]:	178.27
CAS:	88-40-4

Physical Properties

Property code	Value	Unit	Source
gf	41.15	kJ/mol	Joback Method
hf	-218.39	kJ/mol	Joback Method
hfus	13.87	kJ/mol	Joback Method
hvap	47.02	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.301		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	529.79	K	Joback Method
tc	742.25	K	Joback Method
tf	301.11	K	Joback Method
vc	0.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.81	J/molxK	529.79	Joback Method
cpg	392.73	J/molxK	565.20	Joback Method
cpg	408.71	J/molxK	600.61	Joback Method
cpg	423.77	J/molxK	636.02	Joback Method
cpg	437.96	J/molxK	671.43	Joback Method

cpg	451.31	J/molxK	706.84	Joback Method
cpg	463.85	J/molxK	742.25	Joback Method
dvisc	0.0018283	Paxs	301.11	Joback Method
dvisc	0.0009574	Paxs	339.22	Joback Method
dvisc	0.0005713	Paxs	377.34	Joback Method
dvisc	0.0003748	Paxs	415.45	Joback Method
dvisc	0.0002639	Paxs	453.56	Joback Method
dvisc	0.0001962	Paxs	491.68	Joback Method
dvisc	0.0001523	Paxs	529.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	1.30	NIST Webbook

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=C88404&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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