Benzene, 2-methoxy-1,3,5-trimethyl-

Other names:	Anisole, 2,4,6-trimethyl-
	Methoxymesitylene
	2,4,6-Trimethylanisole
	2-methoxy-1,3,5-trimethylbenzene
Inchi:	InChI=1S/C10H14O/c1-7-5-8(2)10(11-4)9(3)6-7/h5-6H,1-4H3
InchiKey:	NNVKEOMPDSKFGZ-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	COc1c(C)cc(C)cc1C
Mol. weight [g/mol]:	150.22
CAS:	4028-66-4

Physical Properties

Property code	Value	Unit	Source
gf	11.84	kJ/mol	Joback Method
hf	-179.83	kJ/mol	Joback Method
hfus	15.72	kJ/mol	Joback Method
hvap	44.53	kJ/mol	Joback Method
ie	8.28	eV	NIST Webbook
log10ws	-3.02		Crippen Method
logp	2.620		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1159.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1170.00		NIST Webbook
ripol	1417.00		NIST Webbook
tb	477.00 ± 3.00	K	NIST Webbook
tc	699.09	K	Joback Method
tf	288.67	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	282.49	J/mol×K	492.24	Joback Method
cpg	296.02	J/mol×K	526.72	Joback Method
cpg	308.99	J/mol×K	561.19	Joback Method
cpg	321.42	J/mol×K	595.67	Joback Method
cpg	333.28	J/mol×K	630.14	Joback Method
cpg	344.60	J/mol×K	664.62	Joback Method
cpg	355.37	J/mol×K	699.09	Joback Method
dvisc	0.0010441	Pa×s	288.67	Joback Method
dvisc	0.0006612	Pa×s	322.60	Joback Method
dvisc	0.0004568	Pa×s	356.53	Joback Method
dvisc	0.0003365	Pa×s	390.46	Joback Method
dvisc	0.0002603	Pa×s	424.38	Joback Method
dvisc	0.0002092	Pa×s	458.31	Joback Method
dvisc	0.0001732	Pa×s	492.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4028664&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ie: Ionization energy
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