

Benzene, 2-methoxy-1,3,4-trimethyl-

Other names:	Anisole, 2,3,6-trimethyl- 2,3,6-Trimethylanisole
Inchi:	InChI=1S/C10H14O/c1-7-5-6-8(2)10(11-4)9(7)3/h5-6H,1-4H3
InchiKey:	MIOQAXCZXWHELT-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	COc1c(C)ccc(C)c1C
Mol. weight [g/mol]:	150.22
CAS:	21573-36-4

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
log10ws	-3.02		Crippen Method
logp	2.620		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1163.00		NIST Webbook
tb	492.24	K	Joback Method
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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21573364&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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