

2,3,4-Trimethylanisole

Other names:	Anisole, 2,3,4-trimethyl
Inchi:	InChI=1S/C10H14O/c1-7-5-6-10(11-4)9(3)8(7)2/h5-6H,1-4H3
InchiKey:	LPWNOAFKRVPOEC-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	COc1ccc(C)c(C)c1C
Mol. weight [g/mol]:	150.22

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
mcpol	133.870	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1139.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1233.00		NIST Webbook
tb	492.24	K	Joback Method
tc	699.09	K	Joback Method
tf	288.67	K	Joback Method
vc	0.505	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.49	J/molxK	492.24	Joback Method
cpg	296.02	J/molxK	526.72	Joback Method
cpg	308.99	J/molxK	561.19	Joback Method
cpg	321.42	J/molxK	595.67	Joback Method
cpg	333.28	J/molxK	630.14	Joback Method
cpg	344.60	J/molxK	664.62	Joback Method

cpg	355.37	J/molxK	699.09	Joback Method
dvisc	0.0010441	Paxs	288.67	Joback Method
dvisc	0.0006612	Paxs	322.60	Joback Method
dvisc	0.0004568	Paxs	356.53	Joback Method
dvisc	0.0003365	Paxs	390.46	Joback Method
dvisc	0.0002603	Paxs	424.38	Joback Method
dvisc	0.0002092	Paxs	458.31	Joback Method
dvisc	0.0001732	Paxs	492.24	Joback Method

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=R142680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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
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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