

3,4-DIMETHYLANISOLE

Other names:	Benzene, 4-methoxy-1,2-dimethyl-
Inchi:	InChI=1S/C9H12O/c1-7-4-5-9(10-3)6-8(7)2/h4-6H,1-3H3
InchiKey:	LVUBSVWMOWKPDJ-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	COc1ccc(C)c(C)c1
Mol. weight [g/mol]:	136.19

Physical Properties

Property code	Value	Unit	Source
af	0.4459		Cheméo Relay (1.0)
gf	13.05	kJ/mol	Joback Method
hf	-131.61	kJ/mol	Cheméo Relay (1.0)
hfus	13.52	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Cheméo Relay (1.0)
ie	7.91	eV	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	2.312		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1123.60		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1164.00		NIST Webbook
tb	477.70	K	NIST Webbook
tb	473.70	K	NIST Webbook
tc	682.04	K	Cheméo Relay (1.0)
tf	252.76	K	Cheméo Relay (1.0)
vc	0.440	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.84	J/mol×K	464.38	Joback Method

cpg	308.18	J/mol×K	672.88	Joback Method
cpg	298.13	J/mol×K	638.13	Joback Method
cpg	287.55	J/mol×K	603.38	Joback Method
cpg	276.44	J/mol×K	568.63	Joback Method
cpg	264.78	J/mol×K	533.88	Joback Method
cpg	252.59	J/mol×K	499.13	Joback Method
dvisc	0.0003782	Pa×s	364.63	Joback Method
dvisc	0.0001853	Pa×s	464.38	Joback Method
dvisc	0.0002266	Pa×s	431.13	Joback Method
dvisc	0.0002865	Pa×s	397.88	Joback Method
dvisc	0.0013208	Pa×s	264.88	Joback Method
dvisc	0.0005277	Pa×s	331.38	Joback Method
dvisc	0.0007933	Pa×s	298.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.70	K	2.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4685476&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
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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