3,5-DIMETHYLANISOLE

Other names:	2,5-Dimethylanisole
	3,5-Dimethylanizole
	Anisole, 3,5-dimethyl
	Benzene, 1-methoxy-3,5-dimethyl-
Inchi:	InChI=1S/C9H12O/c1-7-4-8(2)6-9(5-7)10-3/h4-6H,1-3H3
InchiKey:	JCHJBEZBHANKGA-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	COc1cc(C)cc(C)c1
Mol. weight [g/mol]:	136.19

Physical Properties

Property code	Value	Unit	Source
af	0.4568		Cheméo Relay (1.0)
gf	13.05	kJ/mol	Joback Method
hf	-129.41	kJ/mol	Cheméo Relay (1.0)
hfus	13.52	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Cheméo Relay (1.0)
ie	8.09	eV	Cheméo Relay (1.0)
log10ws	-3.02		Cheméo Relay (1.0)
logp	2.312		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1111.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1120.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1533.00		NIST Webbook
tb	466.20	K	NIST Webbook
tc	672.98	K	Cheméo Relay (1.0)
tf	243.54	K	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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C874635&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point