

2,3-Dimethylanisole

Other names:	Benzene, 1-methoxy-2,3-dimethyl-
Inchi:	InChI=1S/C9H12O/c1-7-5-4-6-9(10-3)8(7)2/h4-6H,1-3H3
InchiKey:	BLMBNEVGYRXFNA-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	<chem>COc1cccc(C)c1C</chem>
Mol. weight [g/mol]:	136.19
CAS:	2944-49-2

Physical Properties

Property code	Value	Unit	Source
gf	13.05	kJ/mol	Joback Method
hf	-147.72	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	41.64	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.312		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1144.20		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1144.20		NIST Webbook
tb	468.20	K	NIST Webbook
tb	472.20	K	NIST Webbook
tc	672.88	K	Joback Method
tf	264.88	K	Joback Method
vc	0.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.84	J/mol×K	464.38	Joback Method
cpg	252.59	J/mol×K	499.13	Joback Method
cpg	264.78	J/mol×K	533.88	Joback Method
cpg	276.44	J/mol×K	568.63	Joback Method

cpg	287.55	J/mol×K	603.38	Joback Method
cpg	298.13	J/mol×K	638.13	Joback Method
cpg	308.18	J/mol×K	672.88	Joback Method
dvisc	0.0013208	Paxs	264.88	Joback Method
dvisc	0.0007933	Paxs	298.13	Joback Method
dvisc	0.0005277	Paxs	331.38	Joback Method
dvisc	0.0003782	Paxs	364.63	Joback Method
dvisc	0.0002865	Paxs	397.88	Joback Method
dvisc	0.0002266	Paxs	431.13	Joback Method
dvisc	0.0001853	Paxs	464.38	Joback Method

Sources

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=C2944492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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