

2,6-Dimethoxytoluene

Other names:	Benzene, 1,3-dimethoxy-2-methyl- 2-Methylresorcinol, dimethyl ether 1,3-Dimethoxy-2-methylbenzene
Inchi:	InChI=1S/C9H12O2/c1-7-8(10-2)5-4-6-9(7)11-3/h4-6H,1-3H3
InchiKey:	FPEUDBGJAVKAEE-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	COc1cccc(OC)c1C
Mol. weight [g/mol]:	152.19
CAS:	5673-07-4

Physical Properties

Property code	Value	Unit	Source
gf	-91.95	kJ/mol	Joback Method
hf	-279.94	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	44.05	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.012		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
ripol	1243.00		NIST Webbook
ripol	1224.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1264.10		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1243.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1783.00		NIST Webbook
tb	486.80	K	Joback Method
tc	693.63	K	Joback Method
tf	287.11	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.85	J/molxK	486.80	Joback Method
cpg	275.38	J/molxK	521.27	Joback Method
cpg	287.43	J/molxK	555.74	Joback Method
cpg	299.00	J/molxK	590.21	Joback Method
cpg	310.08	J/molxK	624.69	Joback Method
cpg	320.65	J/molxK	659.16	Joback Method
cpg	330.70	J/molxK	693.63	Joback Method
dvisc	0.0010774	Paxs	287.11	Joback Method
dvisc	0.0006652	Paxs	320.39	Joback Method
dvisc	0.0004497	Paxs	353.67	Joback Method
dvisc	0.0003252	Paxs	386.95	Joback Method
dvisc	0.0002475	Paxs	420.24	Joback Method
dvisc	0.0001961	Paxs	453.52	Joback Method
dvisc	0.0001604	Paxs	486.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5673074&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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