

3,5-Dimethoxytoluene

Other names:	Benzene, 1,3-dimethoxy-5-methyl- Orcinol dimethyl ether Toluene, 3,5-dimethoxy- 1,3-Dimethoxy-5-methylbenzene 5-Methylresorcinol dimethyl ether 1,5-Dimethoxy-3-methylbenzene 3,5 Dimethoxytoluene (DMT) Orcinol monohydrate, dimethyl ether
Inchi:	InChI=1S/C9H12O2/c1-7-4-8(10-2)6-9(5-7)11-3/h4-6H,1-3H3
InchiKey:	RIZBLVRXRWHLFA-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	<chem>COc1cc(C)cc(OC)c1</chem>
Mol. weight [g/mol]:	152.19
CAS:	4179-19-5

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
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1269.30		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1258.00		NIST Webbook

rinpol	1282.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1276.00		NIST Webbook
ripol	1866.00		NIST Webbook
ripol	1844.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1864.00		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	330.70	J/molxK	693.63	Joback Method
cpg	320.65	J/molxK	659.16	Joback Method
cpg	310.08	J/molxK	624.69	Joback Method
cpg	299.00	J/molxK	590.21	Joback Method
cpg	287.43	J/molxK	555.74	Joback Method
cpg	275.38	J/molxK	521.27	Joback Method
cpg	262.85	J/molxK	486.80	Joback Method
dvisc	0.0010774	Paxs	287.11	Joback Method
dvisc	0.0001604	Paxs	486.80	Joback Method
dvisc	0.0001961	Paxs	453.52	Joback Method
dvisc	0.0002475	Paxs	420.24	Joback Method
dvisc	0.0003252	Paxs	386.95	Joback Method
dvisc	0.0004497	Paxs	353.67	Joback Method
dvisc	0.0006652	Paxs	320.39	Joback Method
hvapt	59.50	kJ/mol	447.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4179195&Units=SI
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

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
hvapt:	Enthalpy of vaporization at a given temperature
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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