

2,4-DIMETHOXYPHENOL

Inchi:	InChI=1S/C8H10O3/c1-10-6-3-4-7(9)8(5-6)11-2/h3-5,9H,1-2H3
InchiKey:	MNVMYTVDDOXZLS-UHFFFAOYSA-N
Formula:	C8H10O3
SMILES:	COc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	154.17

Physical Properties

Property code	Value	Unit	Source
hf	-395.44	kJ/mol	Cheméo Relay (1.0)
hfus	18.29	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Cheméo Relay (1.0)
ie	7.80	eV	Cheméo Relay (1.0)
log10ws	-1.61		Cheméo Relay (1.0)
logp	1.409		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
tb	528.95	K	Cheméo Relay (1.0)
tf	336.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.41	J/mol×K	539.56	Joback Method
cpg	279.41	J/mol×K	576.57	Joback Method
cpg	289.80	J/mol×K	613.58	Joback Method
cpg	299.60	J/mol×K	650.59	Joback Method
cpg	308.87	J/mol×K	687.60	Joback Method
cpg	317.62	J/mol×K	724.61	Joback Method
cpg	325.89	J/mol×K	761.62	Joback Method
dvisc	0.0009897	Pa×s	375.04	Joback Method
dvisc	0.0004960	Pa×s	402.46	Joback Method
dvisc	0.0002715	Pa×s	429.88	Joback Method
dvisc	0.0001597	Pa×s	457.30	Joback Method
dvisc	0.0000998	Pa×s	484.72	Joback Method
dvisc	0.0000656	Pa×s	512.14	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13330659&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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