

2,5-DIMETHYL-PARA-ANISALDEHYDE

Other names:	2,5-Dimethyl-4-methoxybenzaldehyde Benzaldehyde, 4-methoxy-2,5-dimethyl- 2,5-dimethyl-p-anisaldehyde
Inchi:	InChI=1S/C10H12O2/c1-7-5-10(12-3)8(2)4-9(7)6-11/h4-6H,1-3H3
InchiKey:	KYHULTSMPDXSLR-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	COc1cc(C)c(C=O)cc1C
Mol. weight [g/mol]:	164.20

Physical Properties

Property code	Value	Unit	Source
hfus	18.01	kJ/mol	Joback Method
ie	8.28	eV	Cheméo Relay (1.0)
log10ws	-2.42		Cheméo Relay (1.0)
logp	2.125		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
tb	536.05	K	Cheméo Relay (1.0)
tc	757.19	K	Cheméo Relay (1.0)
tf	341.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.74	J/mol×K	540.90	Joback Method
cpg	366.03	J/mol×K	751.75	Joback Method
cpg	356.56	J/mol×K	716.61	Joback Method
cpg	346.53	J/mol×K	681.46	Joback Method
cpg	335.93	J/mol×K	646.32	Joback Method
cpg	324.76	J/mol×K	611.18	Joback Method
cpg	313.03	J/mol×K	576.04	Joback Method
dvisc	0.0004123	Pa×s	435.78	Joback Method
dvisc	0.0002163	Pa×s	540.90	Joback Method
dvisc	0.0002603	Pa×s	505.86	Joback Method
dvisc	0.0003220	Pa×s	470.82	Joback Method

dvisc	0.0011841	Pa×s	330.67	Joback Method
dvisc	0.0005511	Pa×s	400.75	Joback Method
dvisc	0.0007787	Pa×s	365.71	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.20	K	1.60	NIST Webbook

Sources

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
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=C6745751&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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