

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:	<chem>COc1cc(C)c(C=O)cc1C</chem>
Mol. weight [g/mol]:	164.20
CAS:	6745-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-87.68	kJ/mol	Joback Method
hf	-265.41	kJ/mol	Joback Method
hfus	18.01	kJ/mol	Joback Method
hvap	51.25	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.125		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	540.90	K	Joback Method
tc	751.75	K	Joback Method
tf	330.67	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.74	J/molxK	540.90	Joback Method
cpg	356.56	J/molxK	716.61	Joback Method
cpg	346.53	J/molxK	681.46	Joback Method
cpg	335.93	J/molxK	646.32	Joback Method
cpg	324.76	J/molxK	611.18	Joback Method
cpg	313.03	J/molxK	576.04	Joback Method

cpg	366.03	J/molxK	751.75	Joback Method
dvisc	0.0002163	Paxs	540.90	Joback Method
dvisc	0.0002603	Paxs	505.86	Joback Method
dvisc	0.0003220	Paxs	470.82	Joback Method
dvisc	0.0004123	Paxs	435.78	Joback Method
dvisc	0.0005511	Paxs	400.75	Joback Method
dvisc	0.0007787	Paxs	365.71	Joback Method
dvisc	0.0011841	Paxs	330.67	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6745751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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