3-Methoxy-4,5-methylenedioxybenzaldehyde

Other names:	1,3-Benzodioxole-5-carboxaldehyde, 7-methoxy- 3-Methoxypiperonal 7-methoxybenzo-1,3-dioxole-5-carboxaldehyde
Inchi:	InChI=1S/C9H8O4/c1-11-7-2-6(4-10)3-8-9(7)13-5-12-8/h2-4H,5H2,1H3
InchiKey:	LOFRBHZYZCIOJO-UHFFFAOYSA-N
Formula:	C9H8O4
SMILES:	COc1cc(C=O)cc2c1OCO2
Mol. weight [g/mol]:	180.16
CAS:	5780-07-4

Physical Properties

Property code	Value	Unit	Source
gf	-199.88	kJ/mol	Joback Method
hf	-415.63	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	58.26	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.236		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	583.33	K	Joback Method
tc	809.74	K	Joback Method
tf	394.72	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.11	J/mol×K	583.33	Joback Method
cpg	303.68	J/mol×K	621.06	Joback Method
cpg	313.57	J/mol×K	658.80	Joback Method
cpg	322.81	J/mol×K	696.53	Joback Method

cpg	331.43	J/mol×K	734.27	Joback Method
cpg	339.47	J/mol×K	772.00	Joback Method
cpg	346.95	J/mol×K	809.74	Joback Method
dvisc	0.0016780	Pa×s	394.72	Joback Method
dvisc	0.0012589	Pa×s	426.16	Joback Method
dvisc	0.0009825	Pa×s	457.59	Joback Method
dvisc	0.0007916	Pa×s	489.02	Joback Method
dvisc	0.0006547	Pa×s	520.46	Joback Method
dvisc	0.0005532	Pa×s	551.89	Joback Method
dvisc	0.0004761	Pa×s	583.33	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5780074&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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