3-METHOXYPIPERONAL

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

Physical Properties

Property code	Value	Unit	Source
hfus	28.44	kJ/mol	Joback Method
hvap	73.25	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
logp	1.236		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	553.65	K	Cheméo Relay (1.0)
tf	355.95	K	Cheméo Relay (1.0)

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

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=C5780074&Units=SI
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point