METHYL PIPERONYLATE

Other names:	Methyl piperonylate
	Methyl 3,4-methylenedioxybenzoate
	Piperonylic acid, methyl ester
	methyl 1,3-benzodioxole-5-carboxylate
	Methyl piperonate
Inchi:	InChI=1S/C9H8O4/c1-11-9(10)6-2-3-7-8(4-6)13-5-12-7/h2-4H,5H2,1H3
InchiKey:	QCHGUEIECOASJU-UHFFFAOYSA-N
Formula:	C9H8O4
SMILES:	COC(=O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]:	180.16

Physical Properties

Property code	Value	Unit	Source
af	0.5896		Cheméo Relay (1.0)
hf	-536.34	kJ/mol	Cheméo Relay (1.0)
hfus	28.14	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-3.04		Cheméo Relay (1.0)
logp	1.202		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	543.27	K	Cheméo Relay (1.0)
tc	779.86	K	Cheméo Relay (1.0)
tf	357.39	K	Cheméo Relay (1.0)
vc	0.482	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.82	J/mol×K	583.56	Joback Method
cpg	303.96	J/mol×K	622.02	Joback Method
cpg	314.33	J/mol×K	660.48	Joback Method
cpg	323.97	J/mol×K	698.93	Joback Method

cpg	332.92	J/mol×K	737.39	Joback Method
cpg	341.21	J/mol×K	775.85	Joback Method
cpg	348.90	J/mol×K	814.31	Joback Method
dvisc	0.0017880	Pa×s	390.13	Joback Method
dvisc	0.0012966	Pa×s	422.37	Joback Method
dvisc	0.0009841	Pa×s	454.61	Joback Method
dvisc	0.0007747	Pa×s	486.85	Joback Method
dvisc	0.0006282	Pa×s	519.08	Joback Method
dvisc	0.0005221	Pa×s	551.32	Joback Method
dvisc	0.0004428	Pa×s	583.56	Joback Method

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=C326567&Units=SI

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume