

1,3-Benzodioxole-5-carboxylic acid, methyl ester

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:	<chem>COC(=O)c1ccc2c(c1)OCO2</chem>
Mol. weight [g/mol]:	180.16
CAS:	326-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-219.65	kJ/mol	Joback Method
hf	-431.16	kJ/mol	Joback Method
hfus	28.14	kJ/mol	Joback Method
hvap	57.63	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.202		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
rinpol	1932.00		NIST Webbook
rinpol	1932.00		NIST Webbook
tb	583.56	K	Joback Method
tc	814.31	K	Joback Method
tf	390.13	K	Joback Method
vc	0.456	m ³ /kmol	Joback Method

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	Paxs	390.13	Joback Method
dvisc	0.0012966	Paxs	422.37	Joback Method
dvisc	0.0009841	Paxs	454.61	Joback Method
dvisc	0.0007747	Paxs	486.84	Joback Method
dvisc	0.0006282	Paxs	519.08	Joback Method
dvisc	0.0005221	Paxs	551.32	Joback Method
dvisc	0.0004428	Paxs	583.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C326567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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