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: COC(=O)c1ccc2c(c1)OCO2

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	m3/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	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	486.84	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

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/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