3-Methyl-1,4-benzodioxan-2-carboxylic acid, ethyl ester

Inchi: InChI=1S/C12H14O4/c1-3-14-12(13)11-8(2)15-9-6-4-5-7-10(9)16-11/h4-8,11H,3H2,1-2H

InchiKey: JTBHBFGHWBSLFU-UHFFFAOYSA-N

Formula: C12H14O4

SMILES: CCOC(=O)C1Oc2ccccc2OC1C

Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
gf	-212.28	kJ/mol	Joback Method
hf	-528.45	kJ/mol	Joback Method
hfus	36.34	kJ/mol	Joback Method
hvap	63.20	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.778		Crippen Method
mcvol	164.500	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	642.15	K	Joback Method
tc	866.52	K	Joback Method
tf	399.42	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.33	J/mol×K	642.15	Joback Method
cpg	458.72	J/mol×K	679.54	Joback Method
cpg	473.08	J/mol×K	716.94	Joback Method
cpg	486.45	J/mol×K	754.33	Joback Method
cpg	498.85	J/mol×K	791.73	Joback Method
cpg	510.32	J/mol×K	829.12	Joback Method
cpg	520.88	J/mol×K	866.52	Joback Method
dvisc	0.0018051	Pa×s	399.42	Joback Method
dvisc	0.0012220	Pa×s	439.88	Joback Method
dvisc	0.0008834	Pa×s	480.33	Joback Method

dvisc	0.0006717	Pa×s	520.78	Joback Method
dvisc	0.0005313	Pa×s	561.24	Joback Method
dvisc	0.0004337	Pa×s	601.69	Joback Method
dvisc	0.0003632	Pa×s	642.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6006780&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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