Methyl 6-methoxy-2-methyl-3,4-methylenedioxy-benzoate

Inchi: InChI=1S/C11H12O5/c1-6-9(11(12)14-3)7(13-2)4-8-10(6)16-5-15-8/h4H,5H2,1-3H3

InchiKey: DYBGHVJXCODBIL-UHFFFAOYSA-N

Formula: C11H12O5

SMILES: COC(=O)c1c(OC)cc2c(c1C)OCO2

Mol. weight [g/mol]: 224.21

Physical Properties

Property code	Value	Unit	Source
gf	-327.07	kJ/mol	Joback Method
hf	-627.60	kJ/mol	Joback Method
hfus	33.73	kJ/mol	Joback Method
hvap	65.81	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.519		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1643.00		NIST Webbook
tb	661.70	K	Joback Method
tc	882.77	K	Joback Method
tf	459.94	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.38	J/mol×K	661.70	Joback Method
cpg	420.59	J/mol×K	698.55	Joback Method
cpg	432.08	J/mol×K	735.39	Joback Method
cpg	442.86	J/mol×K	772.24	Joback Method
cpg	452.93	J/mol×K	809.08	Joback Method
cpg	462.31	J/mol×K	845.93	Joback Method

cpg	471.00	J/mol×K	882.77	Joback Method
dvisc	0.0010169	Pa×s	459.94	Joback Method
dvisc	0.0007731	Pa×s	493.57	Joback Method
dvisc	0.0006087	Pa×s	527.19	Joback Method
dvisc	0.0004931	Pa×s	560.82	Joback Method
dvisc	0.0004092	Pa×s	594.45	Joback Method
dvisc	0.0003464	Pa×s	628.07	Joback Method
dvisc	0.0002982	Pa×s	661.70	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R273922&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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