Methyl 4-(3,4-methylenedioxyphenyl)butanoate

Inchi: InChI=1S/C12H14O4/c1-14-12(13)4-2-3-9-5-6-10-11(7-9)16-8-15-10/h5-7H,2-4,8H2,1H3

InchiKey: VHUABZULWQQCDI-UHFFFAOYSA-N

Formula: C12H14O4

SMILES: COC(=O)CCCc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
gf	-194.39	kJ/mol	Joback Method
hf	-493.08	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	64.30	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.911		Crippen Method
mcvol	164.500	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1653.00		NIST Webbook
tb	652.20	K	Joback Method
tc	870.40	K	Joback Method
tf	423.94	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.80	J/mol×K	652.20	Joback Method
cpg	494.77	J/mol×K	834.03	Joback Method
cpg	484.53	J/mol×K	797.67	Joback Method
cpg	473.56	J/mol×K	761.30	Joback Method
cpg	461.81	J/mol×K	724.93	Joback Method
cpg	449.24	J/mol×K	688.57	Joback Method
cpg	504.33	J/mol×K	870.40	Joback Method
dvisc	0.0003448	Pa×s	652.20	Joback Method
dvisc	0.0004140	Pa×s	614.16	Joback Method

dvisc	0.0005092	Pa×s	576.11	Joback Method
dvisc	0.0006449	Pa×s	538.07	Joback Method
dvisc	0.0008467	Pa×s	500.03	Joback Method
dvisc	0.0011625	Pa×s	461.98	Joback Method
dvisc	0.0016897	Pa×s	423.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R84007&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