(2E,4E)-Methyl 5-(benzo[d][1,3]dioxol-5-yl)penta-2,4-dienoate

Inchi: InChI=1S/C13H12O4/c1-15-13(14)5-3-2-4-10-6-7-11-12(8-10)17-9-16-11/h2-8H,9H2,1H3

InchiKey: VOZJBFJHMHRLDN-ZUVMSYQZSA-N

Formula: C13H12O4

SMILES: COC(=O)C=CC=Cc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 232.23

CAS: 6190-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-25.53	kJ/mol	Joback Method
hf	-279.28	kJ/mol	Joback Method
hfus	38.90	kJ/mol	Joback Method
hvap	66.45	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.158		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	2081.70		NIST Webbook
rinpol	2081.70		NIST Webbook
tb	683.40	K	Joback Method
tc	915.31	K	Joback Method
tf	425.05	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.74	J/mol×K	683.40	Joback Method
cpg	453.47	J/mol×K	722.05	Joback Method
cpg	465.30	J/mol×K	760.70	Joback Method
cpg	476.31	J/mol×K	799.35	Joback Method
cpg	486.60	J/mol×K	838.01	Joback Method
cpg	496.26	J/mol×K	876.66	Joback Method
cpg	505.37	J/mol×K	915.31	Joback Method

dvisc	0.0013437	Pa×s	425.05	Joback Method
dvisc	0.0008770	Pa×s	468.11	Joback Method
dvisc	0.0006150	Pa×s	511.17	Joback Method
dvisc	0.0004558	Pa×s	554.23	Joback Method
dvisc	0.0003527	Pa×s	597.28	Joback Method
dvisc	0.0002825	Pa×s	640.34	Joback Method
dvisc	0.0002326	Pa×s	683.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6190461&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/83-095-5/2E-4E-Methyl-5-benzo-d-1-3-dioxol-5-yl-penta-2-4-dienoate.pdf
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