4H-Oxocin-5,6-dicarboxylic acid, dimethyl ester, (Z,Z,E)-

Inchi: InChI=1S/C11H12O5/c1-14-10(12)8-4-3-6-16-7-5-9(8)11(13)15-2/h3,5-7H,4H2,1-2H3/b6
InchiKey: BEXZKZFLMYHWDZ-FKOIWDERSA-N
Formula: C11H12O5
SMILES: COC(=O)C1=C(C(=O)OC)CC=COC=C1
Mol. weight [g/mol]: 224.21
CAS: 39622-57-6

Physical Properties

Property code	Value	Unit	Source
gf	-433.64	kJ/mol	Joback Method
hf	-679.23	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.077		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	670.81	K	Joback Method
tc	897.56	K	Joback Method
tf	416.52	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.97	J/mol×K	670.81	Joback Method
cpg	432.55	J/mol×K	708.60	Joback Method
cpg	445.17	J/mol×K	746.39	Joback Method
cpg	456.82	J/mol×K	784.18	Joback Method
cpg	467.47	J/mol×K	821.97	Joback Method
cpg	477.08	J/mol×K	859.76	Joback Method
cpg	485.65	J/mol×K	897.56	Joback Method
dvisc	0.0010001	Pa×s	416.52	Joback Method
dvisc	0.0005474	Pa×s	458.90	Joback Method

dvisc	0.0003317	Pa×s	501.28	Joback Method
dvisc	0.0002173	Pa×s	543.66	Joback Method
dvisc	0.0001514	Pa×s	586.05	Joback Method
dvisc	0.0001107	Pa×s	628.43	Joback Method
dvisc	0.0000842	Pa×s	670.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39622576&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