9,9-Dimethoxybicyclo[3.3.1]nona-2,4-dione

Inchi: InChI=1S/C11H16O4/c1-14-11(15-2)7-4-3-5-8(11)10(13)6-9(7)12/h7-8H,3-6H2,1-2H3
InchiKey: CFBRRDQMCNWXLH-UHFFFAOYSA-N
Formula: C11H16O4
SMILES: COC1(OC)C2CCCC1C(=O)CC2=O
Mol. weight [g/mol]: 212.24
CAS: 117132-08-8

Physical Properties

Property code	Value	Unit	Source
gf	-341.44	kJ/mol	Joback Method
hf	-688.19	kJ/mol	Joback Method
hfus	10.38	kJ/mol	Joback Method
hvap	52.28	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.934		Crippen Method
mcvol	159.010	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	653.42	K	Joback Method
tc	895.58	K	Joback Method
tf	439.61	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.34	J/mol×K	653.42	Joback Method
cpg	481.69	J/mol×K	693.78	Joback Method
cpg	500.06	J/mol×K	734.14	Joback Method
cpg	517.50	J/mol×K	774.50	Joback Method
cpg	534.08	J/mol×K	814.86	Joback Method
cpg	549.86	J/mol×K	855.22	Joback Method
cpg	564.91	J/mol×K	895.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117132088&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
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