4,7-Dimethoxyindan-1-one

Inchi: InChI=1S/C11H12O3/c1-13-9-5-6-10(14-2)11-7(9)3-4-8(11)12/h5-6H,3-4H2,1-2H3
InchiKey: MSGQVFMAKBIPNF-UHFFFAOYSA-N
Formula: C11H12O3
SMILES: COc1ccc(OC)c2c1CCC2=O
Mol. weight [g/mol]: 192.21
CAS: 52428-09-8

Physical Properties

Property code	Value	Unit	Source
gf	-138.87	kJ/mol	Joback Method
hf	-377.25	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	53.63	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.833		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1790.00		NIST Webbook
tb	616.77	K	Joback Method
tc	847.70	K	Joback Method
tf	412.57	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.63	J/mol×K	616.77	Joback Method
cpg	375.94	J/mol×K	655.26	Joback Method
cpg	389.47	J/mol×K	693.75	Joback Method
cpg	402.21	J/mol×K	732.23	Joback Method
cpg	414.16	J/mol×K	770.72	Joback Method
cpg	425.30	J/mol×K	809.21	Joback Method
cpg	435.63	J/mol×K	847.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52428098&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