1,2-Dimethoxy-3-acetoacetylnaphthalene

Inchi: InChI=1S/C14H14O4/c1-9(15)18-12-8-10-6-4-5-7-11(10)13(16-2)14(12)17-3/h4-8H,1-3H
InchiKey: XTBBSNLXDNRMQB-UHFFFAOYSA-N
Formula: C14H14O4
SMILES: COc1c(OC(C)=O)cc2ccccc2c1OC
Mol. weight [g/mol]: 246.26

Physical Properties

Property code	Value	Unit	Source
gf	-186.75	kJ/mol	Joback Method
hf	-448.34	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.782		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	2219.00		NIST Webbook
tb	701.45	K	Joback Method
tc	923.52	K	Joback Method
tf	460.84	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.57	J/mol×K	701.45	Joback Method
cpg	496.21	J/mol×K	738.46	Joback Method
cpg	508.97	J/mol×K	775.47	Joback Method
cpg	520.85	J/mol×K	812.48	Joback Method
cpg	531.85	J/mol×K	849.49	Joback Method
cpg	541.99	J/mol×K	886.51	Joback Method
cpg	551.26	J/mol×K	923.52	Joback Method
dvisc	0.0006398	Pa×s	460.84	Joback Method
dvisc	0.0004661	Pa×s	500.94	Joback Method

dvisc	0.0003559	Pa×s	541.04	Joback Method
dvisc	0.0002821	Pa×s	581.14	Joback Method
dvisc	0.0002304	Pa×s	621.25	Joback Method
dvisc	0.0001928	Pa×s	661.35	Joback Method
dvisc	0.0001647	Pa×s	701.45	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R553090&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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