1,2,3-trimethoxy-naphthalene

Inchi: InChI=1S/C13H14O3/c1-14-11-8-9-6-4-5-7-10(9)12(15-2)13(11)16-3/h4-8H,1-3H3
InchiKey: RANYXVFYAIGDFE-UHFFFAOYSA-N
Formula: C13H14O3
SMILES: COc1cc2ccccc2c(OC)c1OC
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
gf	-66.25	kJ/mol	Joback Method
hf	-315.12	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Joback Method
hvap	57.66	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.866		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	624.70	K	Joback Method
tc	844.29	K	Joback Method
tf	399.64	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.38	J/mol×K	624.70	Joback Method
cpg	430.79	J/mol×K	661.30	Joback Method
cpg	444.42	J/mol×K	697.90	Joback Method
cpg	457.25	J/mol×K	734.50	Joback Method
cpg	469.31	J/mol×K	771.09	Joback Method
cpg	480.58	J/mol×K	807.69	Joback Method
cpg	491.07	J/mol×K	844.29	Joback Method
dvisc	0.0006293	Pa×s	399.64	Joback Method

dvisc	0.0004577	Pa×s	437.15	Joback Method
dvisc	0.0003501	Pa×s	474.66	Joback Method
dvisc	0.0002785	Pa×s	512.17	Joback Method
dvisc	0.0002286	Pa×s	549.68	Joback Method
dvisc	0.0001924	Pa×s	587.19	Joback Method
dvisc	0.0001653	Pa×s	624.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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