

1,2,4-trimethoxy-naphthalene

Inchi:	InChI=1S/C13H14O3/c1-14-11-8-12(15-2)13(16-3)10-7-5-4-6-9(10)11/h4-8H,1-3H3
InchiKey:	WYZRFRHDHZZWIH-UHFFFAOYSA-N
Formula:	C13H14O3
SMILES:	<chem>COc1cc(OC)c2ccccc2c1OC</chem>
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	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	624.70	K	Joback Method
tc	844.29	K	Joback Method
tf	399.64	K	Joback Method
vc	0.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004577	Paxs	437.15	Joback Method
dvisc	0.0003501	Paxs	474.66	Joback Method
dvisc	0.0002785	Paxs	512.17	Joback Method
dvisc	0.0002286	Paxs	549.68	Joback Method
dvisc	0.0001924	Paxs	587.19	Joback Method
dvisc	0.0001653	Paxs	624.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301507&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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